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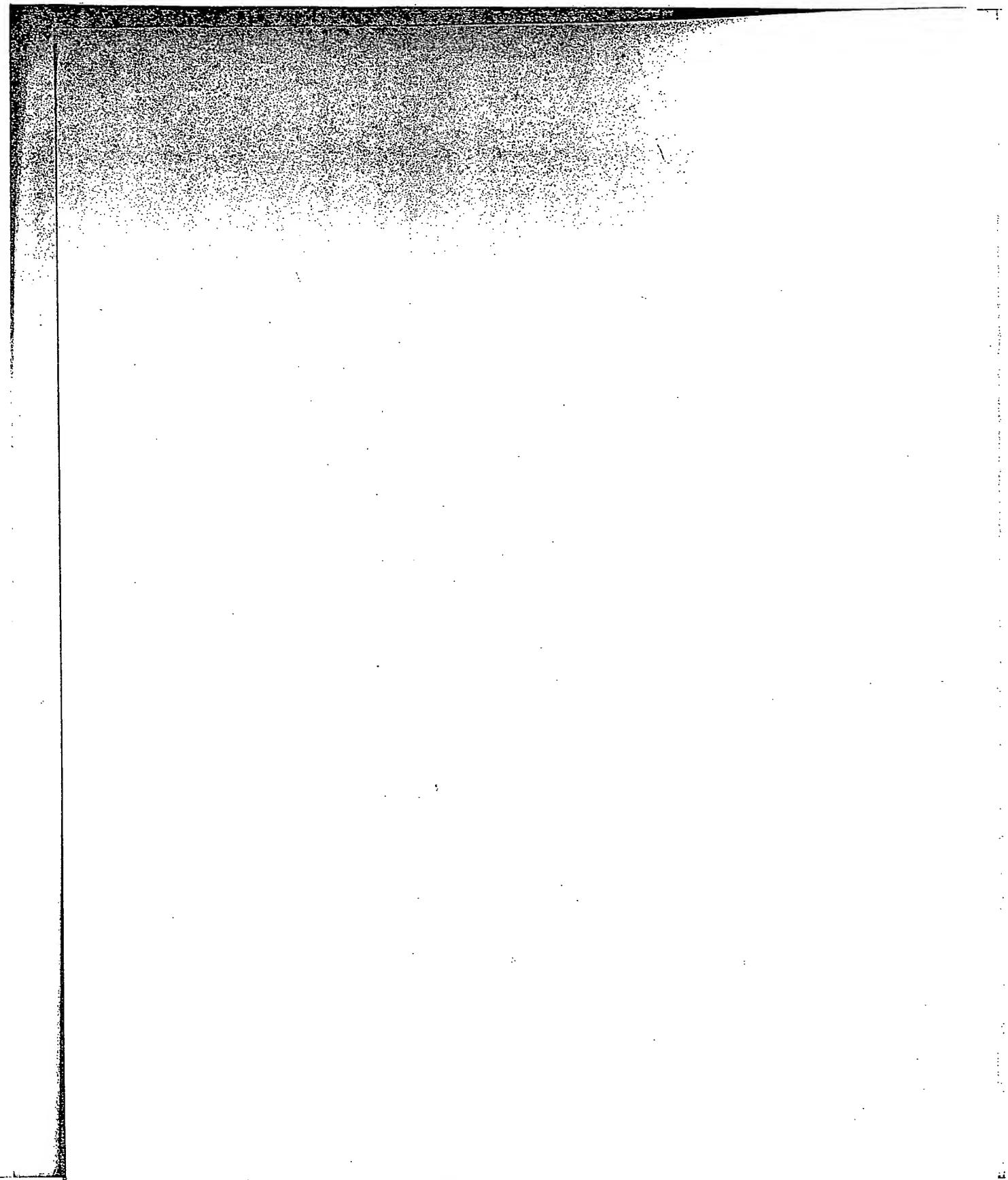
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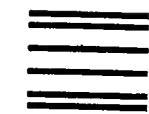
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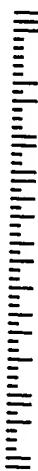
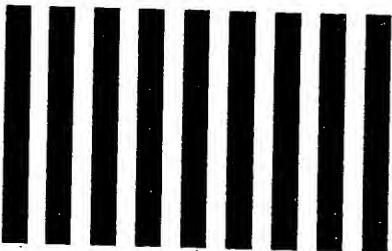
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Desktop Chemistry Software Leader

User's Guide

CS ChemDraw Pro
Version 4.0
for Microsoft Windows and Apple Macintosh

CS ChemDraw Pro is a standalone application within **CS ChemOffice**,
an integrated system including **CS Chem3D** for molecular modeling
and **CS ChemFinder** for searching and chemical information.

ChemDraw

Chemical Structure Drawing Standard

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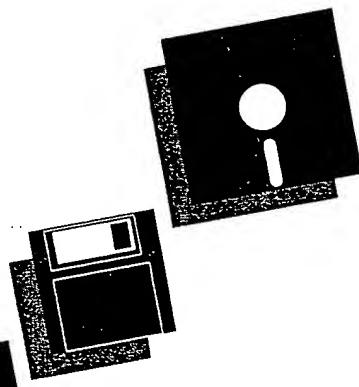
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That makes sense, but what do I get out of purchasing my own software?



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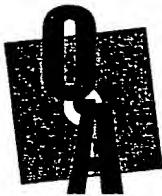
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So I'm never allowed to copy software for any other reason?



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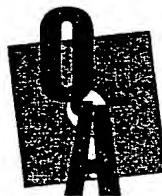
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Many employees don't realize that corporations are bound by the copyright laws, just like everyone else. Such conduct exposes the company (and possibly the persons involved) to liability for copyright infringement. Consequently, more and more corporations concerned about their liability have written policies against such "softlifting". Employees may face disciplinary action if they make extra copies of the company's software for use at home or on additional computers within the office. A good rule to remember is that there must be one authorized copy of a software product for every computer upon which it is run.



Do the same rules apply to bulletin boards and user groups? I always thought that the reason they got together was to share software.

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What about schools and professional training organizations?

The same copyright responsibilities that apply to individuals and corporations apply to schools and professional training organizations. No one is exempt from the copyright law.



I'll bet most of the people who copy software don't even know that they're breaking the law.

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The SPA also offers a number of other materials designed to help you comply with the Copyright Law. These materials include:

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- SPAudit (DOS and Macintosh). This Kit, available free of charge, will audit hard disks to inventory programs and summarize the number and location of each application.
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Introduction

ChemDraw is designed to aid professional scientists and scientific authors in the task of communicating chemical structures. *ChemDraw* employs a straightforward graphical interface. Because *ChemDraw* is designed specifically for communicating chemical structures, *ChemDraw* automatically employs conventions that are intuitive to people who routinely work with chemical structures.

Quite a bit of thought and experimentation has been put into making *ChemDraw* as easy to use as possible while providing superior drawing quality. We hope you find *ChemDraw* a useful tool.

ABOUT THIS USER'S GUIDE

This manual covers CS *ChemDraw* for Windows and Macintosh platforms. The pictures in the manual have been taken from both platforms, and therefore may differ from what you see on your screen.

Documentation for UNIX users

Documentation for the UNIX version of CS *ChemDraw* is provided in an on-line manual (in Adobe Acrobat PDF format). This file is located on the CD that came with your software.

ORGANIZATION OF THIS USER'S GUIDE

The majority of this user's guide is designed in a task-oriented fashion. For example, to learn how to draw a bond, refer to Chapter 3, *Drawing Chemical Structures*. To learn how to position objects in the document window, refer to Chapter 12, *Working with Page Layout*. For basic operations, refer to your operating system documentation.

CONVENTIONS

The following notations are used throughout this user's guide:

 The PRO symbol indicates that a feature is available in CS *ChemDraw Pro* only.

- Instructions are always preceded by a bullet “•” and shown in bold type.

Notes are used throughout this user's guide to highlight information that may be out of context to the current discussion.

■ NOTE:

The following terminology is used throughout this user's guide:

- “Point” refers to moving the mouse until the mouse pointer is over the item you want.
- “Click” refers to quickly pressing then releasing the mouse button.
- “Double-click” refers to clicking the mouse twice in rapid succession.
- “Drag” refers to the following complete action: holding down the mouse button, moving the mouse, and releasing the mouse button.
- “Select” means to highlight an object or choose an option. Selecting something does not initiate an action. However, it marks the item upon which you want to act or provide information. Deselect is the opposite of select.
- “Choose” means to select a command from a menu or submenu, or to click a Toolbar button, or to click a button in a dialog box that completes or cancels a command. Choosing an item performs a command.
- “Key+click” means to hold the specified Key and click the mouse button. For example, Shift+click means hold down the Shift key and click the mouse button.
- “Key+drag” means to hold down the specified key and drag a selection. For example, Shift+drag means to hold down the Shift key and drag the pointer.

GETTING ADDITIONAL HELP

Along with this task-oriented manual, users can find information in the on-line help file.

A Quick Reference card for *ChemDraw* is found at the back of this manual. This card provides summaries to the commands and features for this application. The Quick Reference cards should be used as you run through the tutorials in *Chapter 2, Getting Started Tutorials*, since many of the instructions require the knowledge of elements of the interface.

In the Macintosh version, you can use Balloon help by choosing Show Balloons from the Help menu. Once started, you can point to objects of the *ChemDraw* interface and read short paragraphs about the object as described within the balloon that appears.

Macintosh users running System 7.5 or higher can also use Apple Guide™. We have provided several simple tutorials that guide you through basic techniques for drawing structures.

INSTALLATION/SYSTEM REQUIREMENTS

To install *ChemDraw*, refer to the "Read Me First" document that came with your software. In addition, late breaking news concerning installation can be found in the Read Me file (Macintosh) or Readme.txt (Windows) on your installation disk or CD-ROM.

Windows System Requirements:

ChemDraw runs on most IBM compatible computers having a minimum of a 486 processor. The operating system must be either Windows NT (version 3.5 or later), Windows (version 3.1 or later) or Windows 95.

To run under Windows 3.1 requires a minimum of 8 MB of RAM. In addition, you must install the WIN32s DLLs that come with the installation disks and virtual memory must be turned on.

To run under Windows 95 requires a minimum of 8 MB of RAM and virtual memory turned on.

To run under Windows NT 3.5 requires a minimum of 12 MB of RAM.

You will need a hard drive with at least 10 MB of available disk space.

Macintosh System Requirements:

ChemDraw can run on any Macintosh or Macintosh-compatible computer that supports MacOS version 7.0 or later and has a minimum of 4 MB of RAM.

You will need a hard drive with at least 5 MB of available disk space.

Chapter 1, ChemDraw Basics

This chapter discusses the basic information required to begin using *ChemDraw*. You will learn how to start a session, create, open and save documents, identify the parts of the *ChemDraw* application and customize certain aspects of the user environment.

STARTING CHEMDRAW

You can start the *ChemDraw* application in several ways:

- (Macintosh) From your desktop you can double-click the *ChemDraw* application icon, or select the icon with a single click and choose Open from the File menu.
- (Windows) From the Program Manager, File Manager (Windows 3.1 or NT) or Explorer (Windows 95 and Window NT 4.0) you can double-click the *ChemDraw* application.

In all cases, *ChemDraw* is launched and a new document is created.

WORKING WITH DOCUMENTS

This section deals with issues concerning the creating, opening and saving of *ChemDraw* documents.

Creating Documents

To create a new document:

- From the File menu, choose New.

 **NOTE:** The New Document command in the File menu uses a style sheet (Windows) or stationery pad (Macintosh) with settings that are commonly used for the majority of documents.

To create a new document using a different style sheet (Windows)

- From the File menu, choose Open Special.

- Choose a Style sheet from the list.

A new document is created that has the settings (and objects) stored in the style sheet.

To create a new document using a stationery pad (Macintosh)

- From the Window menu, choose a stationery document.

A new document is created that has the settings (and objects) stored in the stationery pad.

More about style sheets/stationery pads

ChemDraw comes with a number of pre-defined style sheets/stationery pads which are located in the cd_items directory (Windows) or the *ChemDraw* Folder (Macintosh). For example, the ACS-1996 document is pre-configured to create documents that are set with the bond lengths, bond width, spacing and fonts commonly used in the 2-column format within the Journal of the American Chemical Society. A list of the settings stored in these documents is provided in Appendix D, *Document Settings*.

Opening Documents

To open a *ChemDraw* document:

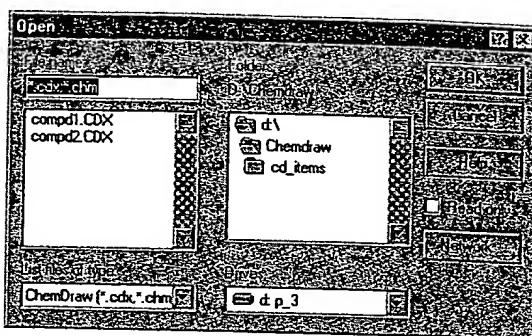
- From the File menu, choose Open

The Open dialog box appears (Figure 1-1)

- Select the location where the file is stored.
- Select the name of the file.
- Click the Open button (Macintosh) or OK button (Windows).

To open a file in a different file format choose the file format of the file from the pop-up menu at the bottom of the dialog box before clicking the Open/OK button. See "Exporting and Importing using File Formats" in Chapter 13, *Sharing Information*, for more information.

Figure 1-1 The Open dialog box



Switching Between Open Documents

Each time you open a document, a document window appears. If you have opened more than one document, the document windows are stacked. The frontmost document is the active window where you can actually do work. All open documents are listed in the Window menu.

There are several ways to make another open document the active window:

- From the Window menu, choose the document.
- Or, click any exposed area of the window you want to be the active window.
- press **Ctrl+Tab** to switch between the currently open document windows (Windows only)

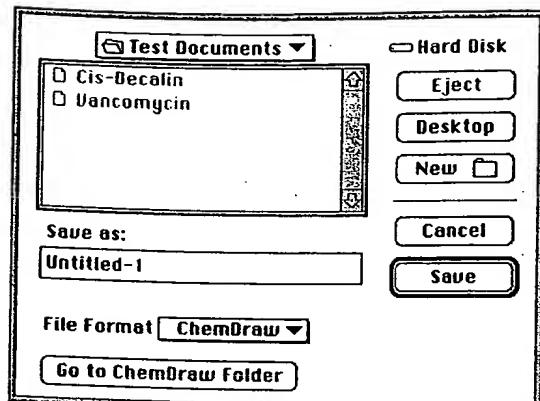
Saving Documents

To save a ChemDraw document:

- From the File menu, choose Save.

The Save dialog box will appear (Figure 1-2).

Figure 1-2 The Save File dialog box



Depending on the platform you are working under, the dialog box will differ. However, the main parts are present in all. The dialog shown above is from the Macintosh version of ChemDraw.

NOTE: In the Macintosh version, there is also a Go To ChemDraw Folder button. For further details, see "The ChemDraw Folder" later in this chapter.

NOTE: ChemDraw (*.cdx) is the native format that ChemDraw recognizes as its own. As such, all information about the structure will be accurately stored. Other file formats may drop information because of those formats internal structure. For instance, under Windows, saving a file as EPS will remove the chemical significance of the connection between atoms and bonds, and store only a picture of the structure. EPS files in Windows do not store a preview.

- Type a name for the file in the box named "File Name" (Windows) or "Save Current Document As" (Macintosh).

The Macintosh, Windows 95 and Windows NT operating systems allow you to type up to 32 characters for a file's name including spaces (for example, "my first structure in ChemDraw"). However, if you are using the Windows 3.1 operating system you must type a name using the 8.3 convention (for example, "myfile.cdx").

- Choose a directory (folder) in which to store the file.
- Click the Save button (Macintosh) or OK button (Windows) to create the file.

When you save a document in the native *ChemDraw* file format the name of the window changes to the name that you typed indicating that a file has been created in the location that you specified.

NOTE: If you are saving in a different file format, that file is exported to the location you indicated. The document name remains as the name of the document saved in the native file format. See Chapter 13, *Sharing Information*, for more information.

Even though you have now created a physical file for storing information, you still must save your work frequently. Any new information that you add to the window is stored in your computer's memory (RAM) until you again save it.

To save a window that has previously been saved:

- From the File menu, choose Save.

The contents of the file will be updated with the information currently in the window. The dialog will not be displayed.

Saving a Document with a Different Name or Location

You can use the Save As command to save a copy of your document under a different name, save a copy to a different location, or save a copy using a different file format. Saving a copy under a different name or location is useful for keeping earlier revisions of your document. Saving a file as a different type is useful for creating style sheets/stationery pads and for exporting information to other applications.

To save a copy of a *ChemDraw* document under a different name or in a different location:

- From the File menu, choose Save As.
- Type a new name of the file in the Save dialog box and/or choose a new location in which to save.

- Click the OK button (Windows) or Save button (Macintosh).

Saving a Document in a Different File Format

To save a *ChemDraw* document as another file format:

- From the File menu, choose Save As.

The Save As dialog box appears.

- Select a file format from the File Format pop-up menu or from the Save File as Type drop-down list box.
- Type a name for the document in the File Name box.
- Select a directory/folder and disk in which to save the document.
- Click the OK button (Windows) or Save button (Macintosh)

Be aware that if you type a name that already exists for a document that is in the same directory, it will replace the existing version of the document. It is best to use a different name so you do not replace the original *ChemDraw* document. For a discussion of other file formats, see Chapter 13, *Sharing Information*.

The original document in the *ChemDraw* format remains in the active window. The file in the other format is saved with the name and in the location you specified. You should consider saving files in other formats only when they are at a stage where they are complete, not in progress.

Discarding Recent Changes to a Structure

To retrieve the last saved version of a file:

- From the File menu, choose Revert.

All changes made to the file since it was saved last are discarded and the previous version of the file appears.

NOTE: You can use the Undo command in the Edit menu to remove each individual action since the last save.

NOTE: In all ASCII text file formats, the front to back ordering of atoms and bonds are saved in the file, rather than the order in which they were drawn.

Viewing the Location of a Document (Macintosh only)

To view the folder(s) where the document in the frontmost window is located:

- Point to the name of the document in the title bar.
- Hold the Command key down and press the mouse button.

A pop-up menu appears describing the location of the document. The second item in the pop-up menu is the name of the folder (or the disk if there are no folders) that contains the document. The last item in the pop-up menu is the name of the disk that contains the document.

Figure 1-3 Location of a *ChemDraw* Document



To switch to a folder in the listing:

- Select a folder or disk from the pop-up menu.

The folder you chose becomes the active window. The *ChemDraw* document is in the background.

To return to your *ChemDraw* document:

- Click in the window containing your document or choose *ChemDraw* from the Application Icon menu to make it the active application.

The *ChemDraw* document is moved into the active window.

Closing Documents

When you are finished with a document you can close the document window, and file it away.

To close the active window:

- From the File menu, choose Close or double-click the Control-menu box (Windows) or the Close box (Macintosh) in the upper left corner of a document window.

The document in the active window is closed. If you have made any changes to this document since last opening or saving, you will be asked if you want to save the document before closing the window.

Accessing Documents Quickly

You can quickly access *ChemDraw* documents using the *ChemDraw* Folder (Macintosh) and the cd_items directory (Windows).

The *ChemDraw* Folder (Macintosh)

The *ChemDraw* Folder is a special folder that is normally located in the same folder as your *ChemDraw* application (however, it can also be located in the Preferences Folder within your System Folder).

ChemDraw documents contained within the *ChemDraw* Folder are automatically added to the Windows menu. This is useful for accessing documents that you commonly use, such as stationery pads (and Template documents and Template stationery pads in *ChemDraw Pro*).

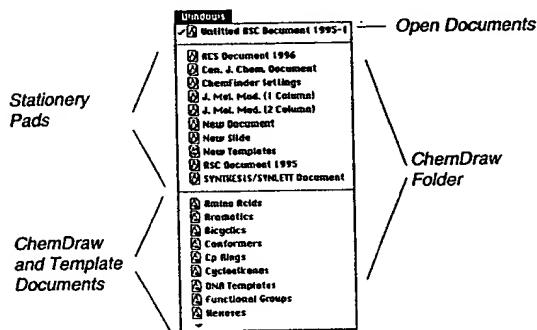
Other files contained within the *ChemDraw* Folder, include the *ChemDraw* Preferences file, scripts, *ChemDraw* HotKeys file, the *ChemDraw* Nicknames file, the isotopes file and the generic nicknames file. However, these files do not appear in the Windows menu (scripts appear in the Scripts menu).

NOTE: You can place aliases of template files or stationery pads in your *ChemDraw* Folder. The originals can come from another folder on your computer or another computer that is on your network. You can then access the alias from the Windows menu.

The Windows Menu (Macintosh Only)

The Windows menu contains two groups of documents: Those currently open and those located in the *ChemDraw* Folder. Choosing any of the documents in the Windows menu performs the same function as opening the same document by one of the standard methods discussed earlier in this chapter. For instance, choosing an open document will make that document the active window. Choosing a stationery pad will open an untitled document based on that stationery pad, and so on. The following illustration shows the various types of documents that may appear in the Windows menu, and the order in which they appear.

Figure 1-4 Organization of the Windows menu



Document types are listed in segments within the Windows menu. Documents within each segment are listed alphabetically. The first segment contains documents that are currently open, both *ChemDraw* documents and Template documents. The open document that is the active window has a checkmark next to it. The second segment lists all stationery pads contained within the *ChemDraw* Folder, both *ChemDraw* stationery and Template stationery pads. The third segment lists any other *ChemDraw* documents or Template documents contained within the *ChemDraw* Folder. The icons for each of the document types are slightly different so that you can distinguish among them.

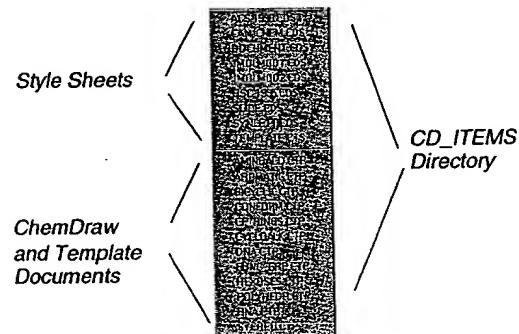
NOTE: **PRO** The Template documents and Template stationery pads only appear in *ChemDraw Pro*.

The cd_items directory (Windows only)

The cd_items directory is a special directory, usually located in the same directory as the *ChemDraw* application (however, it can also be located within the system directory within the Windows directory - see *Appendix B, Specifying Paths* to alter the path to the cd_items folder.).

ChemDraw documents located within this directory are accessible from the Open Special submenu in the File menu. This is useful for accessing documents that you commonly used, such as style sheets (and Template documents and Template style sheets in *ChemDraw Pro*). The organization of the Open Special submenu is shown below in Figure 1-5:

Figure 1-5 Organization of the Open Special submenu



Other files contained within the cd_items directory include the *ChemDraw* Preferences file, *ChemDraw* HotKeys file (hotkeys.txt), *ChemDraw* Nicknames file (nickname.dat), the Isotopes table (isotopes.txt) and the generic nicknames file (generics.txt). However, these files do not appear in the Open Special submenu.

The Window Menu (Windows only)

The Window menu lists all open *ChemDraw* documents (and open Template documents, in *ChemDraw Pro*). In addition, the Window menu contains other standard Windows commands for organizing your document windows and icons within the Application window, such as tiling and cascading. Choosing a document from the Window menu performs the same function as opening the same document by one of the methods discussed earlier in this chapter. The document you choose becomes the active window.

PRINTING

ChemDraw uses the standard system commands to print *ChemDraw* documents. The options that you have available to you will depend on the printer that you are using. You should refer to your printer's documentation for these specifics. In general however, to print a *ChemDraw* document:

- From the File menu, choose Page Setup (Macintosh) or Print Setup (Windows).

Make all appropriate selections for the printer you are using and click the OK button.

- From the File menu, choose Print.
- Make your selections in the Print dialog box and choose the Print button.

Alternatively, to print a document from the File Manager or from the Finder:

- Select the document you want to print.
- From the File menu, choose Print.

The *ChemDraw* application is opened and the Print dialog box appears.

- Make your selections in the Print dialog box and choose the Print button.

Preferences Guide

Print Background Color

You can control whether the Background Color contained in your *ChemDraw* document is printed.

To change whether the Background Color is printed:

- From the File menu, choose Preferences.
- Click the Print Background Color check box.
- Click the OK button.

This change affects all documents.

NOTE: You can specify whether the Background Color contained in your *ChemDraw* document is printed by selecting or deselecting the Print Background Color option in the Preferences dialog box.

(Macintosh) If you are transferring information to another application from which you will print *ChemDraw* pictures, you will need to consider including PostScript commands and the *ChemDraw* LaserPrep File with the pictures. To learn about the special situation to consider, refer to "Transferring PostScript" in Chapter 13, *Sharing Information*.

Print Quality

(Macintosh) When you print a document, *ChemDraw* creates both a QuickDraw representation and a PostScript representation of the document's contents.

QuickDraw is the graphical format that is supported by the Macintosh Operating System. Every printer to which you can print from a Macintosh can convert QuickDraw representations into printed output. However, because QuickDraw is supported by all printers, it does not offer good support for features (like high-resolution printing) that are available only on some printers.

Preferences Guide (Macintosh)

Optimize Pictures for High-Resolution Non-PostScript Printing

Several years ago, Apple enhanced the way the clipboard behaves to better support high-resolution printers. This method uses a High Resolution Clipboard and while it still is QuickDraw based, it can offer much better output quality.

Although ChemDraw supports the use of this High-Resolution Clipboard, it also needs to be supported in the program *into* which you are pasting your pictures. Besides *ChemDraw*, some programs that support the High Resolution Clipboard include PageMaker, MacDraw, KaleidaGraph, and IGOR Pro. Microsoft Word (through version 6.0, at least) is a prime example of a program that does *not* support the High-Resolution Clipboard.

If you are unsure if the application uses a High Resolution Clipboard, try transferring pictures with this checkbox selected and deselected and see which picture prints with higher quality. In addition, if you are printing to a non-PostScript printer, deselect the checkboxes labeled "Include *ChemDraw* LaserPrep" and "Include PostScript" to reduce the size of each picture by 11K to 12K.

To use the High Resolution Clipboard:

- From the File menu, choose Preferences.
- Click the Optimize Pictures for High-Resolution Non-PostScript Printing checkbox.
- Click the OK button.

If you are printing to a PostScript printer, you should turn on the Include PostScript option instead. PostScript will always offer the highest-quality output. For more information, see "Transferring PostScript" in Chapter 13, *Sharing Information*.

This change affects all documents.

The PostScript representation is used by printers that use the PostScript page definition language, such as the Apple LaserWriter NT, and most brands of phototypesetters. The PostScript representation describes objects precisely by using mathematical shapes that can be precisely imaged at whatever resolution is used by your printer. The PostScript representation created by *ChemDraw* is composed of two parts, the PostScript commands and the *ChemDraw* Laser Prep. The *ChemDraw* Laser Prep contains specific instructions that enable the printer to interpret the PostScript commands contained in a *ChemDraw* document.

Preferences Guide (Macintosh)

Include PostScript

If you are transferring *ChemDraw* pictures to another document that will be printed on a PostScript printer:

- From the File menu, choose Preferences.
- Select the Include PostScript checkbox, then click the OK button.

When Include PostScript is not checked, no PostScript commands are generated. This will usually result in lower quality printing, particularly of drawings cut and pasted into other applications. However, since the representation used for printing when Include PostScript is not selected is the same as that used for drawing to the screen, better correspondence between the screen and printed output might be observed in some cases.

Include ChemDraw LaserPrep

Select this checkbox for maximum flexibility when printing to PostScript printers. If you do not select this checkbox, you will need to choose the Initialize LaserWriter command from within *ChemDraw* before you print. If you create pictures with this off and then give them to a colleague, they will be unable to print them to PostScript printers unless they also own a copy of *ChemDraw* and can choose the Initialize LaserWriter command themselves.

For more information, see "Transferring PostScript" in Chapter 13, *Sharing Information*.

QUITTING/EXITING

Quitting an application frees up the memory the application uses so that other applications can have more memory available to them. To close the *ChemDraw* application:

- From the File menu, choose Quit *ChemDraw* (Macintosh) or Exit *ChemDraw* (Windows).

If you have document windows open that have not been saved, you are first asked if you want to save them before you close the application.

CHEMDRAW'S GRAPHICAL INTERFACE

One of the best things about *ChemDraw* is the simplicity of its interface (the part of the application that you interact with to perform tasks). The interface consists of a document window, menus, commands, a tools palette. These items are described below.

Document Window

The central part of the document window contains the work space where you will draw your structures. The Tools palette contains icons for tools that change the way the pointer (cursor) behaves.

The basic components of a *ChemDraw* document window are shown below.

Figure 1-6 The *ChemDraw* document window

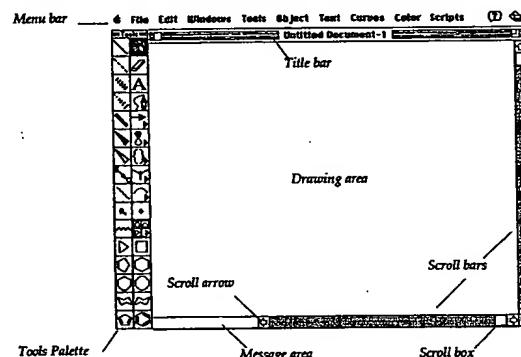


Table 1-1 Parts of the document window

Screen Element	Use
Drawing area	The area within a document window where you can draw.
Menu bar	Contains all the commands specific to the <i>ChemDraw</i> application for manipulating documents and their contents.
Message area	Contains short information messages that appear as you draw, such as the length and angle of bonds or the magnification of the window.
Scroll arrows	Scrolls a document window in small increments in the direction of the arrow.
Scroll bars	Scrolls a document window in large increments.
Scroll boxes	Scrolls a document window in the direction that you drag the box.

Table 1-1 Parts of the document window (*continued*)

Screen Element	Use
Title bar	Contains the name of the application or document as a Window Title. Also, the Title bar can be dragged to move a window. (Macintosh) Holding down the Command key and pressing and holding down the mouse button over the title displays the location of the <i>ChemDraw</i> document.
Tools palette	Contains icons representing the drawing tools available in <i>ChemDraw</i> . Click a tool icon to select it. The selected tool determines what drawing operation is carried out when you click in a document window. You can move the Tools palette by dragging its Title bar.

The Tools Palette

The Tools Palette (Figure 1-7) contains the tools that you can use to draw in a document window. Tools are selected by clicking a tool icon. One tool in the Tools palette is always selected. Tools with a small triangle in the lower right corner contain a palette of choices for the tool. Holding down the mouse button over this type of tool displays the palette. A description of each tool is found in Table 1-2.

Figure 1-7 Tools Palette

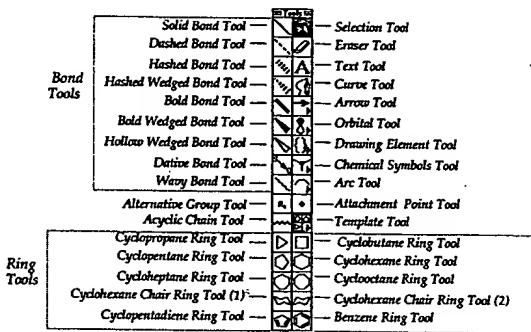


Table 1-2 Tools in the Tools window

Tool Name	Use
Bond Tools	Used for drawing single, double and triple bonds of various types.
Acyclic Chain Tool	Used for quickly drawing chains of any length.
Arc Tool	Used for drawing arcs. Arcs of different degrees can be selected from the Arc Tool's palette.
Alternative Group Tool	In <i>ChemDraw Pro</i> , this tool is used to create alternative group definitions (R, G, etc) that represent a set of substituents, any one of which will match the query.
Attachment Point Tool	In <i>ChemDraw Pro</i> , this tool is used to specify attachment point in an alternative group definition.
Arrow Tool	Used to draw arrows. Arrows of different types can be selected from the Arrow Tools palette.
Chemical Symbols Tool	Used to draw chemically significant symbols such as charges, radicals and lone pairs.

Table 1-2 Tools in the Tools window (continued)

Tool Name	Use
Drawing Elements Tool	Used to draw objects common to reaction schemes, such as brackets and lines. Drawing Elements of different types can be selected from the Drawing Element Tools palette.
Eraser Tool	Used to delete objects.
Orbital Tool	Used for drawing orbitals. Orbitals of different types can be selected from the Orbital Tools palette.
Ring Tools	Used for quickly drawing common structural components.
Pen Tool	Used to draw freehand shapes such as custom arrows and orbitals.
Selection Tool	Used to select objects. Objects that are selected can be further manipulated using menu commands.
Template Tool	Used for drawing structures using templates stored in template documents. Templates can be selected from the Template Tools palette.
Text Tool	Used to create atom labels and captions.

Menus and Commands

The menus in the menu bar contain the commands that you use to perform tasks on a document.

There are several ways to access commands within menus. The three possibilities available in *ChemDraw* are:

1. Mouse: You can display the commands in a menu by pointing to a menu name, hold down the mouse button and drag to the command you want to choose. On Windows, you may alternatively point to the menu name, click it to select and open the menu, then point to the command you want to choose and click the mouse button.

2. Alt, letter, letter: (Windows only) Press the Alt key and then press the underlined letter in the menu name you want to open, release this key and press the underlined letter in the command you want to choose. For example, Alt, F, X opens the File menu and chooses the Exit *ChemDraw* command. If you open a menu and decide not to choose a command you can press the Alt or ESC key to close the menu, or use an Arrow key to open another menu.

3. Command shortcuts: Many commands have keyboard equivalents that you can memorize and use to execute a command directly without first opening the menu. For example on Macintosh, **⌘N** is equivalent to choosing New from the File menu and under Windows, Alt+F4 is equivalent to opening the File menu and choosing Exit *ChemDraw*. The available command key equivalents are listed next to the menu commands.

The appearance of the commands in a menu may change. The different appearances of commands are described in Table 1-3.

Table 1-3 Appearance of commands

Menu Convention	Meaning
Checkmark next to a command	The command is currently turned on, or in effect. Usually, selecting the command again removes the check mark.
✓ Fixed Lengths	
Partial Selection marks next to several commands ► Plain Ctrl+T ► Bold Ctrl+B ► Italic Ctrl+I	Indicates that each selected command applies to part of the current selection (these appear as hyphens under Macintosh)

Table 1-3 Appearance of commands (continued)

Menu Convention	Meaning
Dimmed command (grayed out command) Cut	The command is not available for the current selection, or for the state of the active document.
Ellipsis (...) after a command 	A dialog box appears which requires user input before the command is executed.
Key combination next to a command Group	You can use the command key combination to execute the command rather than choosing it from the menu.
Triangle next to a command 	Indicates that if you press and hold down the mouse button on the name of the command, a submenu with further options appears.

Using Dialog Boxes

Dialog boxes appear when additional information is required to complete commands.

Within a dialog box, there are several ways to navigate:

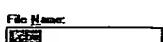
- Mouse:** You can click an option to select it, or click a command button to complete or cancel a command.
- Keyboard:** To move within the dialog box you can press the Tab key to go to the next button or option group, or you can press Shift+Tab to move back to the last button or option group. Option groups and their navigation techniques are discussed in the table that follows.

The different options available are described in Table 1-4.

Table 1-4 Options in dialog boxes

Option Type	Use
Check Boxes 	Check boxes are selected when an "x" appears in the box. You can select as many check boxes as you need. Check boxes without an "x" are deselected.
Drop-down List Boxes or Pop-up Menus 	Drop-down list boxes (Windows) or pop-up menus (Macintosh) provide a list of possible options from which you can choose, much like the menus in the menu bar.
Command Buttons 	Command buttons generally are used to execute the information, or to cancel any changes made. Common command buttons are the OK and Cancel buttons.
Option Button or Radio Button 	In most dialog boxes, a default button exists for executing the command, for example the OK button. The default button has a bolder outline and can be chosen by pressing the Return key.
Spin Button or Control Arrows 	Spin buttons (Windows) or Control Arrows (Macintosh) provide a range of values from which you can select. To select a value, click the up or down arrow on the spin button, or type a value in the text box next to the spin button.

Table 1-4 Options in dialog boxes (continued)

Group	Use
Text Box 	A text box is used to enter textual information, such as a file name. To enter information within a text box, simply point to the box and click to select the text in the box. Next, type the necessary information.

Undoing Actions

ChemDraw keeps track of the actions you perform. You can reverse actions one at a time by choosing the Undo command. The number of actions that can be undone or redone is limited only by the amount of memory (i.e., RAM and virtual memory) available for use by *ChemDraw*. When you save your document the Undo queue is reset and starts over.

To undo the last action performed:

- From the Edit menu, choose Undo.

The last action performed is reversed. The Redo command changes to reflect the undone action. The Undo command changes to reflect the next action you can undo.

For example, if you draw cyclohexane, create an atom label text box, type a label, and select and rotate the structure, you will be able to remove the actions as follows:

1. Remove the rotation.
2. Remove atom label.
3. Remove the ring.

At each step, the Undo command is appended with the action being removed.

Redoing Actions

When you undo an action, the Redo command becomes active. You can reverse the effect of the Undo command by choosing the Redo command. The Redo command is appended with the action being redone.

To redo the last action performed:

- From the Edit menu, choose Redo.

The last action undone is reinstated. The Undo command changes to reflect the next action you can undo. The Redo command changes to reflect the next action that can be redone.

CUSTOMIZING YOUR ENVIRONMENT

In *ChemDraw* there are many ways to customize your work. Preferences allow you to change the default behavior of certain options that will be in force for every open document. Document Settings allow you to change the default behavior of options that will affect only the frontmost document. In addition, you can customize your menus by adding commands that perform tasks using other applications by adding Scripts (Macintosh) or through menu extension DLLs (Windows).

Preferences

Preferences affect the way the *ChemDraw* application works, regardless of the document with which you are working. Preferences affect things like the units of measurement that you use. Preferences are saved in the *ChemDraw* Preferences file (Macintosh) or chemdraw.ini (Windows) which is located within the Windows directory (Windows) or Preferences folder in the System Folder (Macintosh). As you become familiar with the application, you can change the preferences to suit your needs. Preferences are described as the topic to which they apply is discussed.

Figure 1-8 The Preferences dialog box

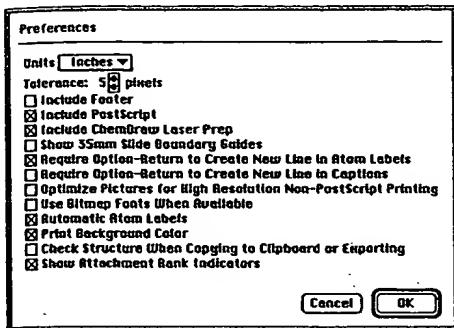


Table 1-5 Preferences options

select this preference..	if you want to...
Units	change the units used in the Drawing Settings dialog box, the Rulers and the Crosshair. Available units include inches, centimeters and points.
Tolerance	change the size of the highlight box that appears when you point at any object in the document window. The tolerance affects how close the cursor needs to be for selecting or joining.
Include Footer	print a footer containing the document name, date and time of the last revision. The footer appears in the lower left corner of a printed document.
Include PostScript (Macintosh only)	transfer <i>ChemDraw</i> pictures to other applications that will eventually print to a PostScript printer. <i>ChemDraw</i> pictures can be transferred through any of the following: the Clipboard, Publish or EGO. If you are printing to a non-PostScript printer, you can leave this checkbox unchecked.
select this preference..	if you want to...
Include ChemDraw Laser Prep Pictures (Macintosh only)	print to a printer that cannot be initialized using <i>ChemDraw</i> (for instance, a service bureau). You should also check the Include PostScript option if you select this option. If you are printing to a non-PostScript printer, there is no need to have this checkbox checked.
Show 35mm Slide Boundary Guides	<p><i>NOTE:</i> This extra PostScript information will add an extra 11 to 12K per picture to the destination document; however it insures that the document containing the <i>ChemDraw</i> pictures can be printed. This affects Clipboard, Publish, EGO, and EPS files.</p> <p>display boundary guides to help you keep your picture in the appropriate ratio for the 35 mm slide format.</p> <p>Boundary lines appear at 7 inches and 10.5 inches. The page size must be at least 7 x 10.5 inches for the boundary guides to appear. The boundary guides are not printed.</p> <p><i>NOTE:</i> This option to print slides is merely an assistant to keeping your structures within the bounds of the standard 35 mm slide dimensions.</p>

Table 1-5 Preferences options (continued)

select this preference...	if you want to...	select this preference...	if you want to...
Require Ctrl-Enter to Create New Line (Windows) or Require Option + Return to Create New Line (Macintosh)	use the Enter key (or Return key for Macintosh users) to close text boxes. When this option is selected, you will need to hold down the Ctrl key and press the Enter key (or the Option and Return key for Macintosh users) to add a new line.	Check Structure When Copying	invoke the Check Structure command when a structure is copied to the Clipboard or saved. This provides a safety check for structures that you will be importing into other applications, such as ISIS/Base.
Optimize Pictures for High Resolution Non-PostScript Printing (Macintosh only)	transfer <i>ChemDraw</i> pictures to another application that uses a High Resolution Clipboard and will be printing the document to a non-PostScript (QuickDraw) printer. If you are unsure if the application uses a High Resolution Clipboard, try transferring pictures with this checkbox selected and deselected and see which picture prints with higher quality.	Show Attachment Rank Indicators	show visual indication of the attachment point ordering in alternative groups.
Use Bitmap Fonts When Available (Macintosh only)	display text on screen using Bitmap fonts rather than TrueType fonts. The text will appear more quickly, and for some fonts, such as Helvetica, the on-screen display is more readable. However, TrueType fonts print more accurately.		
Automatic Atom Labels	have <i>ChemDraw</i> calculate the best alignment for atom that you create. If you want all atom labels to be justified flush left when created, deselect this check box.		
Print Background Color	print the background color. With this option deselected, the background will always print as white.		

Document Settings

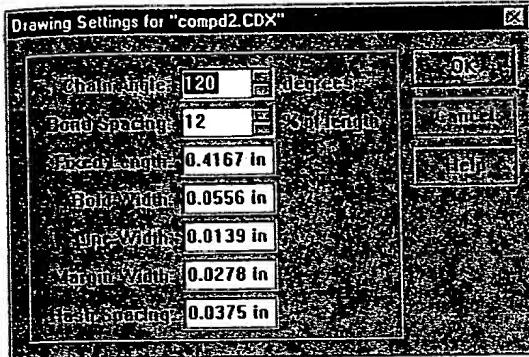
Document settings are user definable settings that are applied to the current document. Document settings include Drawing Settings, Caption Text Settings, Label Text Settings, Print/Page Setup, and the Color Palette. Drawing Settings affect drawing related options such as the fixed length used to draw bonds. Text Settings affect text related options like the font used for atom labels and captions. The Color Palette affects the colors available to Colorize objects. The Print/Page Setup affects options like the page size used.

As you become familiar with *ChemDraw* you can change these settings to fit your needs. You can also save different sets of document settings in style sheets/stationery pads to be used for special instances, such as journal articles, textbook chapters, slide presentations and so on. See "Saving Customized Settings" in Chapter 1, *ChemDraw Basics*, for more information.

Drawing Settings

Drawing Settings are document settings that affect how bonds are drawn. Changes made in the Drawing Settings dialog box (Figure 1-9) take effect for all bonds already drawn as well as those that are drawn later. Changes made affect the active document window only. Drawing settings can be saved in style sheets/stationery pads.

Figure 1-9 Drawing Settings dialog box



A summary of each of the options is described in table 1-6 below:

Table 1-6 Drawing Settings options

Adjust this setting...	If you want to...
Chain Angle	<p>change the angle (from 1 to 179 degrees) between bonds created by the Acyclic chain tool or modified by the Clean Up Structure command</p> <p>For more information see more information see "Acyclic Chain Tool" in Chapter 3, <i>Drawing Chemical Structures</i> and "Structure Clean Up" in Chapter 8, <i>Advanced Drawing Techniques</i>.</p>
Bond Spacing	<p>change the distance between the lines in double or triple bonds. The distance is set as some percentage of the total length of the bond (between 1 and 100). This allows for proportional spacing to be used if different bond lengths are used in the drawing. For more information see "Drawing Settings for Bonds" in Chapter 3, <i>Drawing Chemical Structures</i>.</p>
Fixed Length	<p>constrain the length of the bonds drawn to the length you specify whenever the command Fixed Lengths in the Tools menu is selected (a checkmark is next to it). This will also adjust the preferred bond length for structures modified by the Clean Up Structure command.</p> <p>For more information see "Fixed Lengths" in Chapter 3, <i>Drawing Chemical Structures</i> and "Structure Clean Up" in Chapter 8, <i>Advanced Drawing Techniques</i>.</p>
Bold Width	<p>change the width of the line used when bold and wedge bonds are drawn.</p> <p>For more information see "Drawing Settings for Bonds" in Chapter 3, <i>Drawing Chemical Structures</i>.</p>
Line Width	<p>change the width of all bonds, lines and arrowheads in the drawing.</p> <p>For more information see "Drawing Settings for Bonds" in Chapter 3, <i>Drawing Chemical Structures</i>.</p>
Margin Width	<p>change the amount of space surrounding all atom labels that will erase portions of the bonds to which they are attached. The margin width also determines the amount of white space surrounding the front bonds in a bond crossing.</p> <p>For more information see "Atom Labels" in Chapter 4, <i>Captions and Atom Labels</i>, and "Bond Crossings" in Chapter 3, <i>Drawing Chemical Structures</i>.</p>

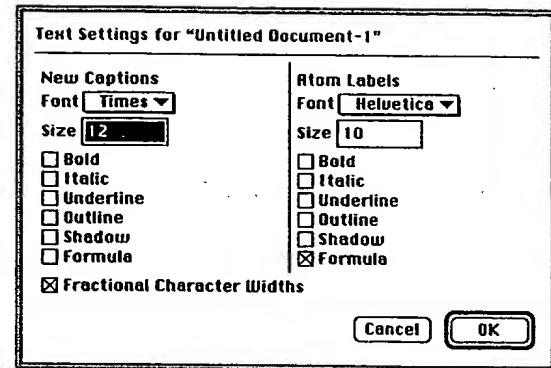
Table 1-6 Drawing Settings options (*continued*)

Adjust this setting...	If you want to...
Hash Spacing	change the spacing between the hashed lines used when wedged hashed bonds, hashed bonds, dashed bonds, dashed arrows or dashed curves are drawn. For more information see "Drawing Settings for Bonds" in <i>Chapter 3, Drawing Chemical Structures</i> .

Text Settings

Text Settings (Macintosh) or Caption Text Settings and Label Text Settings (Windows) affect how new captions and all atom labels for the current document are drawn and formatted. Changing the Text Settings in the Text Settings dialog box (Macintosh, Figure 1-10), or Caption/ Label Text Settings (Windows, Figure 1-11), affects the current document only. You can change the caption Font, Size and Style, and the atom label Font, Size and Style. All captions created after exiting the Text Settings dialog box will use the new settings. All atom labels previously drawn will change in proportion to the new atom label settings. You can save text settings in stationery pad documents (Macintosh) or Style Sheets (Windows) if you repeatedly use the same settings. See *Chapter 4, Captions and Atom Labels*, and "Saving Customized Settings" later in this chapter.

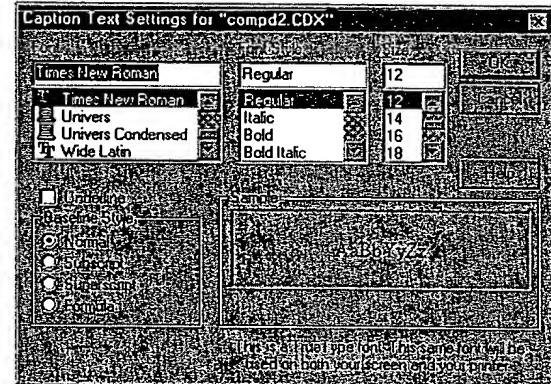
Figure 1-10 Text Settings dialog box (Macintosh)



Fractional Character Widths (Macintosh Only): Choose the Fractional Character Widths checkbox to change the spacing between characters so that they are as close to proportional spacing as possible. If you are printing to a PostScript printer this option generally improves the font appearance. The screen image of the font is also affected by this checkbox, and the text may look irregular on the screen.

NOTE: If you copy structures to other applications, make sure the character widths setting is the same in the other application or else printing problems may occur.

Figure 1-11 Caption Settings dialog box (Windows)

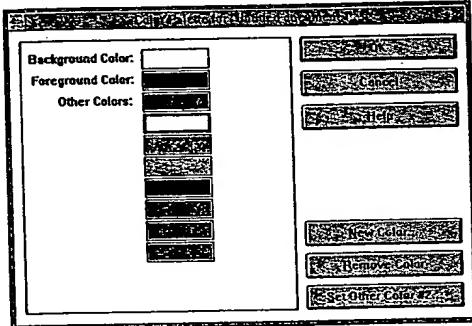


Color Palette

Choose Color Palette to display a dialog box (Figure 1-12) where you can add, remove, or change the default foreground and background color and specify the other colors available for coloring objects. For more information, see "Changing the Color palette" in Chapter 11, *Working with Color*.

Changes made to the color palette affect the current document only. You can save Color Palette settings in a style sheet/stationery pad. For more information see "Saving Customized Settings" later in this chapter.

Figure 1-12 Color Palette dialog box



A summary of each of the options is described in Table 1-7.

Table 1-7 Color Palette options

Click this button	If you want to...
New Color	add a new color box and set its color using the Color Picker or Color Wheel dialog box.
Set Color	change the color associated with a color box that you have selected in the left side of the dialog box. Any objects using the old color are changed to the new color.
Remove Color	delete a color box that you have selected in the left side of the dialog box. Any objects using the removed color are changed to the Foreground color.

Saving Customized Settings

Every new document created within *ChemDraw* uses a style sheet/stationery pad to obtain its document settings. Style Sheets/Stationery Pads can also contain predefined objects. When you create a new document, you actually create an untitled copy of the style sheet/stationery pad. You can make any changes you want to the copy of the style sheet without affecting the style sheet/stationery pad itself. By creating different style sheets/stationery pads, you can avoid the need to specify the document settings repeatedly when you switch between projects that require different settings. As a convenience, style sheets/stationery pads can be stored in the cd_items directory (Windows) or *ChemDraw* Folder (Macintosh) so that they are accessible from the Open Special submenu in the File menu.

Applying Settings From Other Documents

To apply document settings to the active window that are contained in a style sheet located in the cd_items directory/*ChemDraw* Folder:

- From the File menu, choose **Apply Settings**.
- From the **Apply Settings** submenu, choose a style sheet/stationery pad.

The settings in the active document window change to those found in the style sheet/stationery pad that you choose.

To apply the document settings contained in a *ChemDraw* document or style sheet/stationery pad not contained in the cd_items directory (Windows) or *ChemDraw* Folder (Macintosh) to the document in the active window:

- From the **Apply Settings** submenu, choose **Other**. The Open dialog box appears.
- Select a *ChemDraw* document or style sheet/stationery pad and click the **OK** or **Open** button.

NOTE:  In ChemDraw Pro, Template Style Sheets/Stationery Pads don't appear in the Apply Settings pop-up menu. However, you can access Template Style Sheets/Stationery using the Other command.

Scripts (Macintosh Only)

The Scripts menu contains scripts that you can use to perform tasks within ChemDraw or between ChemDraw and another scriptable application.

Scripts found in the Scripts menu are created using Apple's *Script Editor* application. With the proper script extensions in conjunction with Apple's *Script Editor* application, you can create scripts using the AppleScript™ scripting language and add scripts to the Scripts menu by placing them in the ChemDraw Folder.

NOTE: Scripts not stored within the ChemDraw Folder are not accessible from the Scripts menu.

To read about the scripts that come with ChemDraw:

- From the Scripts menu, Choose Read About ChemDraw.

To learn more about AppleScript™ and the *Script Editor* application see your system manuals. There is also a variety of manuals and guides available from various sources that discuss AppleScript™ in more detail.

NOTE: The Scripts menu will not be active if you do not have any Scripts within your ChemDraw Folder. AppleScript 1.1 or later is required to use the scripts supplied with ChemDraw.

Menu Extension DLLs (Windows Only)

Through the ChemOffice SDK (Software Developers Kit), new menus and menu items that control ChemDraw can be added to ChemDraw. At this time, the SDK requires a solid working knowledge of C programming for implementing these menu extensions.

For more information about the SDK see our web page at: <http://www.camsoft.com>.

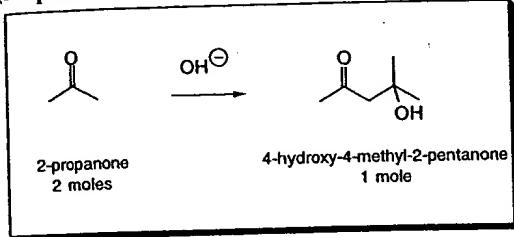
Chapter 2, Getting Started Tutorials

This chapter provides several tutorials designed to teach you useful drawing techniques.

You should review the section "Conventions" in the Introduction of this user's guide. The terminology found there is used throughout these tutorials. You may also find it useful to have your Quick Reference card handy as you perform each tutorial.

TUTORIAL 1: REACTION SCHEMES

In this tutorial, you will draw the following (simplified) reaction scheme:

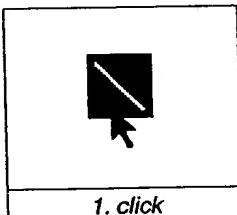


- First, start *ChemDraw*.
- From the File menu, choose Save As.
- In the text box at the bottom of the dialog box, type "tut1.cdx".
- Select a directory (Windows) or folder (Macintosh) in which to save the file.
- Click the OK button (Windows) or the Save button (Macintosh).
- Open the Tools menu and make sure there is a check mark next to the Fixed Lengths and Fixed Angles command. If either command is not checked, choose the command again to select it.

Tools	
Show Crosshair	Ctrl+H
Show Belers	F11
✓ Fixed Lengths	Ctrl+L
✓ Fixed Angles	Ctrl+E

NOTE: Applying fixed lengths and fixed angles assists you in creating structures with bond lengths and angles that are consistent with each other. The fixed length is set in the Drawing Settings dialog box. The fixed angle is always an increment of 15 degrees.

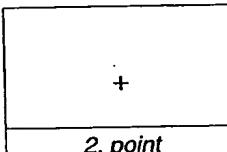
- Select the Solid Bond tool by clicking its icon.



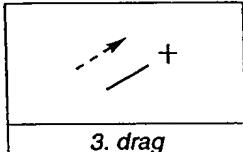
1. click

- Position the pointer (which appears as a cross when a bond tool is selected) anywhere in a document window and hold down the mouse button.

- Drag the mouse diagonally upwards to the right.



2. point



3. drag

Release the mouse button when you have made a 30 degree angle and extended the bond to its fixed length (look at the Message area at the lower left corner of the document window).

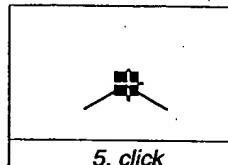
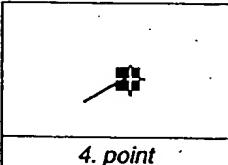
NOTE: When drawing with bond tools, you must always draw the first bond in a structure by dragging as shown above. You cannot begin a structure by clicking using a bond tool or by adding a bond to a caption. If you are using a ring tool, you can click to begin a structure.

Next, add a bond:

- Point to the right atom of the bond.
- Click the atom to add a bond.

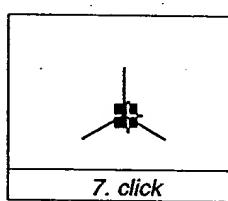
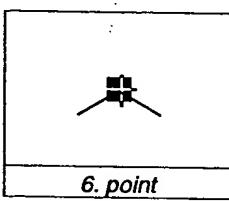
A second bond is deposited forming a 120 degree angle between the bonds.

NOTE: The angle used when clicking to add bonds is controlled by the Chain Angle setting in the Drawing Settings dialog box in the File menu. If this bond angle cannot be established, the next smaller and logical bond angle is used.



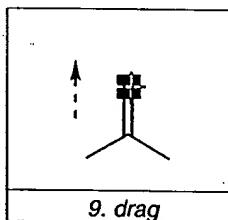
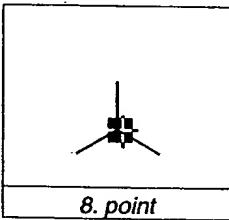
Next, add a second bond:

6. Continue pointing to atom C2.
7. Click the atom to add a bond.



Next you will change a single bond into a double bond:

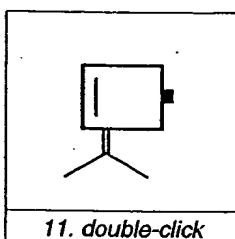
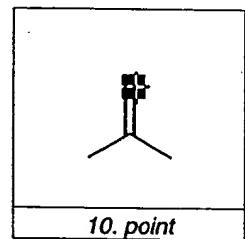
8. Point to C2 and hold the mouse button down.
9. Drag from C2 to C4 over the existing single bond. Release the mouse button.



Next you will add labels to the structure. Atom labels can be added in several ways. These will be illustrated in various steps in the tutorial.

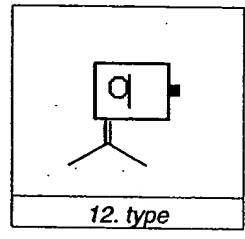
10. Point to atom shown below.

11. Double-click the atom.



12. Type "O" in the text box that appears.

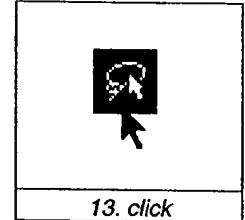
To close the text box you can click in an empty area of the window or click another tool to select it.



In the next series of steps you will learn how to duplicate a structure and create another structure from the duplicate.

First, you will select the structure:

13. Select the Selection tool by clicking its icon.

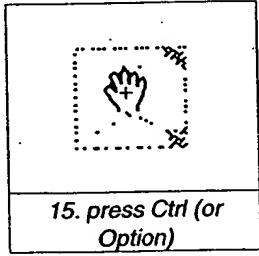
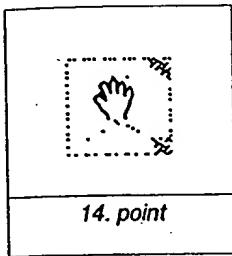


The last structure drawn is automatically selected. Next, you will create the duplicate.

14. Point over the Selection rectangle.

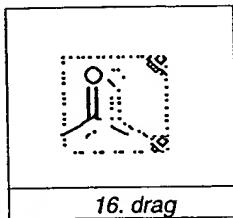
15. Press and hold down the Ctrl key (Windows) or the Option key (Macintosh).

The pointer turns to a hand with a plus sign inside to signal that you are in the duplication mode of the Selection tool.



16. Drag the Selection Rectangle to the right.

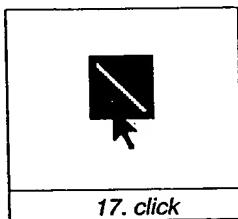
A copy of the structure is created when you begin dragging. The original structure remains in its original position. Release the mouse button when the copy is clear of the original.



TIP: When you create a copy in the manner just shown you can drag it anywhere in the document window. However, you may want to restrict the position of the copy so it remains aligned with the original. To do so, simply hold down the Alt key (Windows) or Command key (Macintosh) in addition to the modifier key mentioned in the last step.

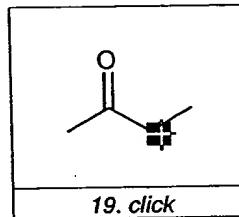
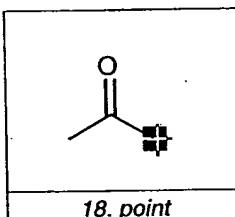
Next, you will modify the duplicated structure.

17. Select the Solid Bond tool by clicking its icon.



18. Point to atom shown below.

19. Click the atom to add a bond.

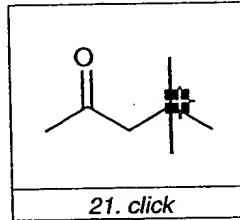
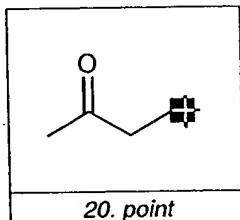


To add several bonds to a single atom:

20. Point to the atom shown below.

21. Click the bond three times, allowing a pause in between each click.

NOTE: If you click too fast, the click will be interpreted as a double-click, and a text box will open, or a triple-click which will repeat your last atom label.

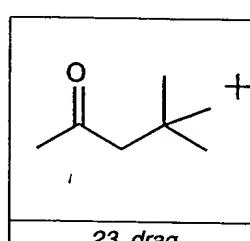
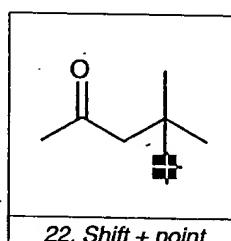


NOTE: The angle used when bonds are deposited in this way is based on the Chain Angles Setting in the Drawing Settings dialog box. If that value cannot be established the next chemically logical angle is used. If you need to reorient one of the bonds that you created, hold down the Shift key and point to a non-attached atom and drag the atom to another position.

To reposition one of the bonds:

22. Hold down the Shift key and point at the vertical bond that is facing downwards.
23. Drag the bond so that it is facing diagonally to upwards to the right.

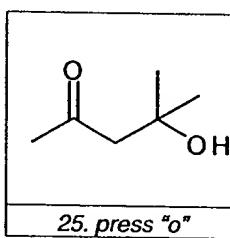
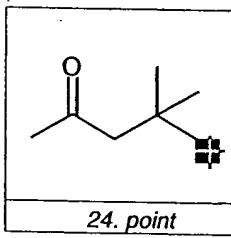
Release the mouse button and depressed keys.



Next you will create an atom label using one of the easiest methods, HotKeys. Many of the keys on your keyboard have been preassigned to be HotKeys and are linked to specific atom labels.

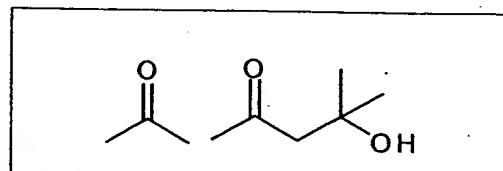
24. Point to atom shown below.
25. Press the lowercase "o" key on your keyboard.

When you use HotKeys that represent a single element, like "O", the proper number of hydrogens are added to the label. To see this, click the double bond with the Eraser tool. To continue with this tutorial, choose Undo from the Edit menu.



In the next step you will move the structures using the Selection tool to make room for adding an arrow. A new method for selecting is introduced.

At this point in the tutorial you should have two structures within your window.

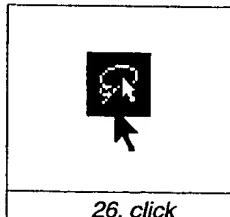


TIP: Now that you have all the structures for the reaction scheme, you can check that you have drawn them correctly by using the Check Structure command.

- Select the Selection tool. The last structure drawn is automatically selected. To select a different structure, double-click one of its bonds.
- Choose Check Structure from the Object menu. A message indicating whether errors were found or not will appear.
- Repeat for the other structure.

NOTE: If an error is found, you can click the Stop button in the message window that appears to highlight the troubled portion of the structure.

26. Select the Selection tool by clicking its icon.

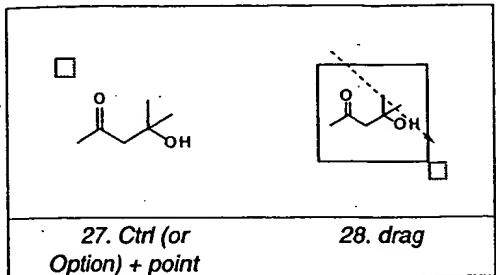


27. Hold down the Ctrl key (Windows) or Option key (Macintosh).

The pointer changes to a box indicating that you are in the Marquee mode of the Selection tool.

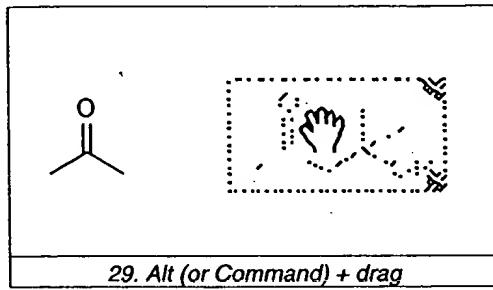
28. Drag diagonally over the entire structure.

Once you have dragged over the objects, release the mouse button and the depressed keys to create the selection.



Next, you will drag the selection to make room for adding an arrow.

29. Hold down the Alt key (Windows) or Command key (Macintosh) to constrain movement of the selection and drag the Selection Rectangle.



Next you will add arrows to a reaction scheme.

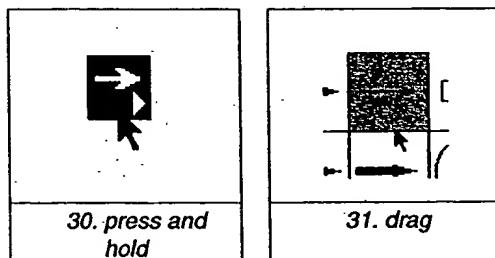
30. Hold down the mouse button over the Arrow tool to display the Arrow palette.

NOTE: The triangle in the lower left corner of the Arrow icon indicates it contains a palette.

31. Drag the cursor to the small normal arrow (first row, third column).

Once you have selected an arrow you can release the mouse button.

NOTE: Once you have chosen an arrow from the palette it becomes the default arrow type. You can use that arrow by clicking the Arrow tool to select it. You only need to display the arrow palette if you want to change to a different arrow type.



Next you will draw using the arrow you selected.

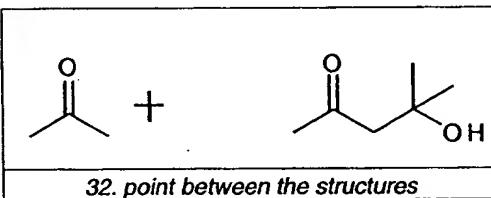
32. Point to the end of the reactant and hold the mouse button down.

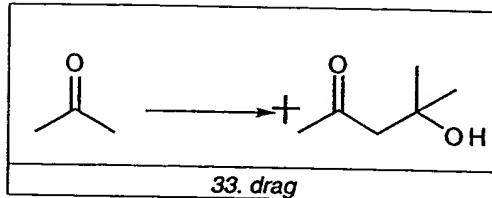
33. Drag the Arrow to the length you want.

When you have the length you want, you can release the mouse button.

Tip: If you need to alter the length (or the angle relative to the X axis) of the arrow after you draw it:

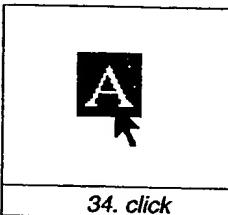
- Hold down the Shift key and point to the arrowhead (a highlight box appears when you are pointing correctly).
- Drag the arrowhead to the length (and angle) you want.





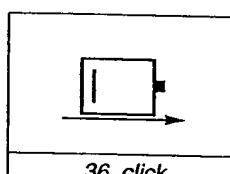
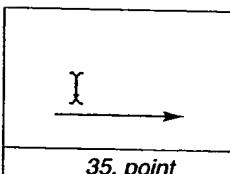
Adding line formula or other captions for representing reagents and/or reaction conditions is performed using the Text tool. As pointed out earlier, the Text tool has two functions, labeling atoms and creating captions. To use the Text tool for creating captions and line formula, point to an empty area of the document window (i.e. don't point at an atom). The pointer will appear as an insertion point indicating that a caption will be created if you click the mouse button.

34. Click the Text tool to select it.

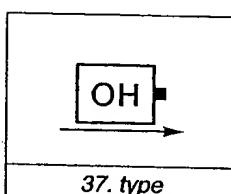


35. Point above the arrow.

36. Click to create a text box.



37. Type "OH".



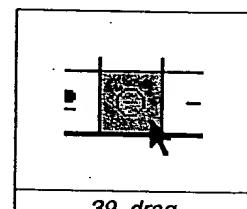
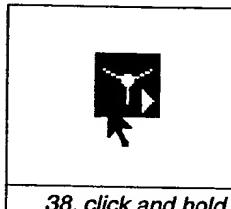
NOTE: Captions and line formula with subscript numbers can be created by choosing the Formula style from the Text menu. In addition, formula style allows you to calculate information about a caption using the Analyze Structure command.

NOTE: To realign the caption if necessary, select the Selection tool and drag the caption.

Next you will add a charge symbol. Rather than add a negative charge symbol using the keyboard, there are specialized symbols available in the Reaction Mechanism tool palette.

38 Click and hold down the mouse button over the Chemical Symbol tool.

39 Hold down the mouse button and drag to the circled negative charge symbol (second row, fourth column) and release the mouse button.

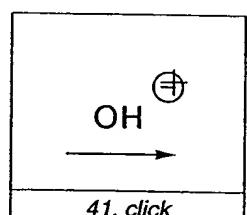
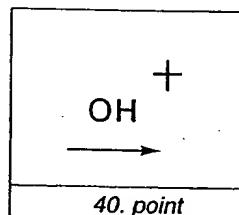


Next you will draw a symbol using the one you selected from the palette:

40 Position the pointer to the right of the OH caption.

41 Click to deposit the charge symbol.

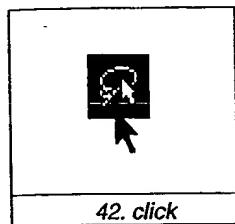
Move the cursor away from the symbol after you have drawn it.



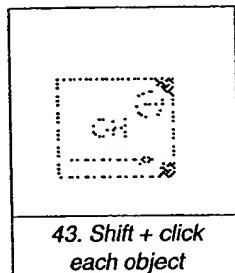
It is often convenient to make several related objects selectable by double-clicking for purposes of manipulating or moving. Any objects added from the Chemical Symbols palette is automatically associated with the structure (or caption in formula style) that it is closest to. However, objects such as arrows are not associated automatically. You can manually group objects using the Group command.

To group several objects:

42. Select the Selection tool by clicking its icon.



43. Hold down the Shift key and click the arrow, the OH caption and the charge symbol.



The Shift key allows you to add objects to a selection without deselecting other objects.

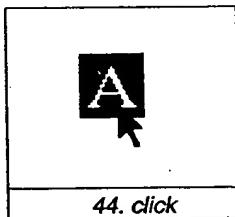
NOTE: If you are holding down the Shift key and click an already selected object, that object is deselected.

- From the Object menu, choose Group.

NOTE: Objects within a group are still selectable as individual objects by single clicking.

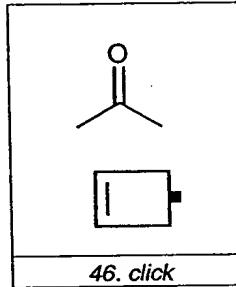
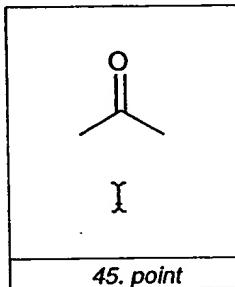
Next, you will use the Text tool to create a caption containing the name and amount of reactant, and center the information under the structure.

44. Click the Text tool to select it.



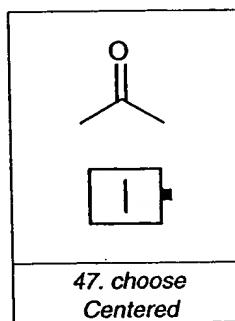
45. Point below your first structure.

46. Click to create a text box.



47. From the Text menu, choose Centered.

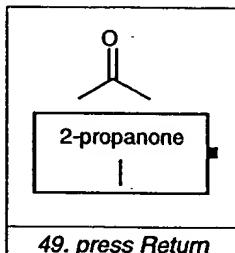
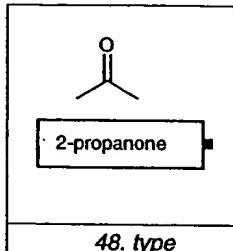
The orientation of the "I" beam changes to the center of the text box (Macintosh). The default that appears whenever you create a new text box is flush left.



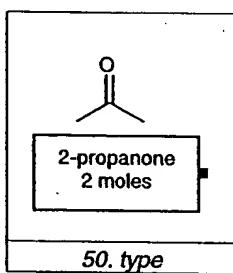
Next, type your caption:

48. Type "2-propanone".

49. Press the Return key to begin a new line.



50. Type "2 moles".

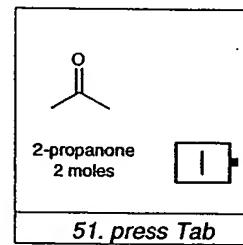


Next you will create an aligned caption for the other structure.

51. Press the Tab key to create another Text box that is aligned adjacent to the first.

52. Type "4-hydroxy-4-methyl-2-pentanone", press Return and type "1 mole".

NOTE: Using the Tab key in the caption mode of the text tool provides a way of creating tables of captions. As an added benefit, the font, size and style (not the justification which is flush left by default) are maintained from the previous caption.



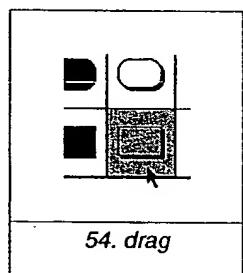
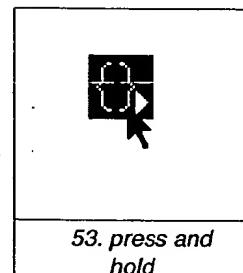
TIP: If your captions are not aligned properly beneath the structures you should move them using the Selection tool.

- Click the Selection tool to select it. The text box is automatically selected since this was the last object you drew.
- Press the Left or Right Arrow key to move the caption so it is centered beneath structures. This method will maintain the alignment created by the Tab key.

To complete the presentation, you can add a shadowed box around the scheme:

53. Hold down the mouse button over the Drawing Elements tool.

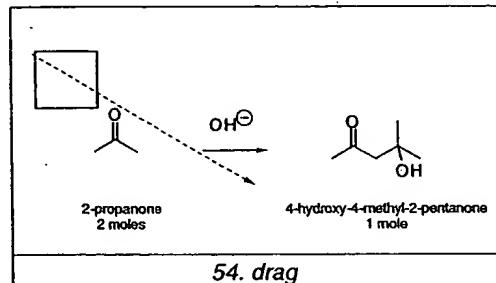
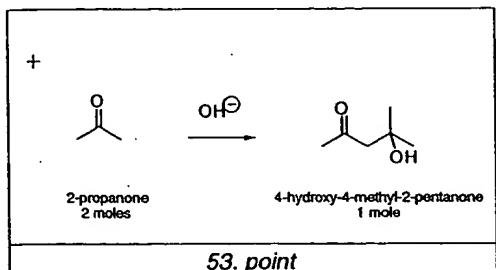
54. Select the shadowed box from the palette of drawing elements.



53. Point to the upper left corner of the reaction scheme.

54. Hold down the mouse button and drag diagonally downward to the left to draw the box.

When the box encompasses the entire reaction scheme release the mouse button.



- From the File menu, choose Save.

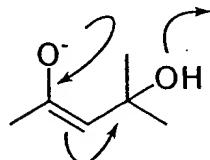
Your changes are saved.

- From the File menu, choose Close.

You have completed your first reaction scheme. In the next exercise you'll add an intermediate to make the scheme more complete.

TUTORIAL 2: DRAWING AN INTERMEDIATE

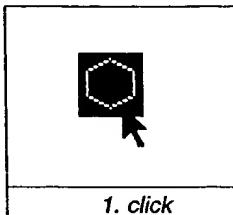
This tutorial will show you how to draw the following intermediate structure starting from a ring and add arrows with customized shapes using the Pen tool:



- From the File menu, choose New Document.
- From the File menu, choose Save As.

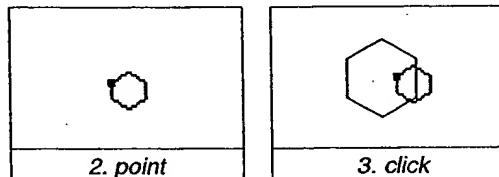
- In the text box at the bottom of the dialog box, type "tut2.cdx".
- Select a directory (Windows) or folder (Macintosh) in which to save the file.
- Click the OK button (Windows) or the Save button (Macintosh).

1. Select the Cyclohexane Ring tool.



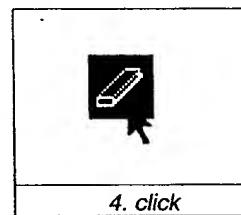
2. Point in an empty area of a document window.

3. Click to deposit a ring.



Next you will erase some of the bonds in the ring:

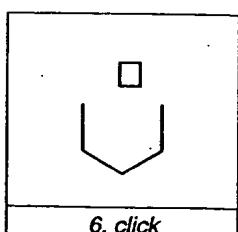
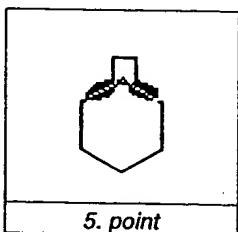
4. Select the Eraser tool.



5. Point to the atom between the apex bonds.

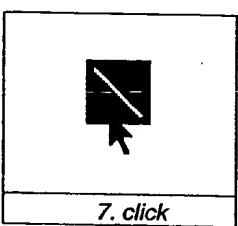
TIP: You can also delete these bonds individually by pointing at the center of a bond and clicking.

6. Click the atom to delete the atom and its bonds.



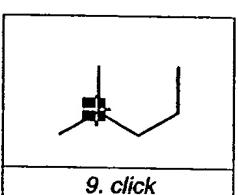
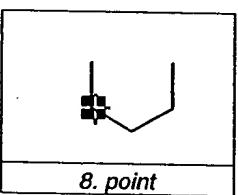
Next you will add a bond:

7. Select the Solid Bond tool.



8. Point to atom C2.

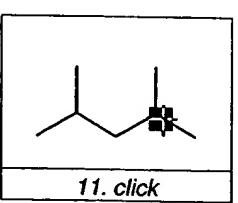
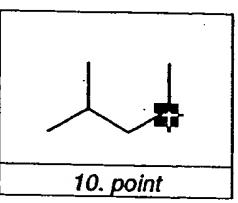
9. Click to add a bond.



Next you will add a second bond:

10. Move the cursor over C4.

11. Click to add another bond.

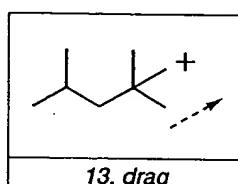
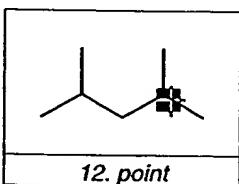


Next you will add a third bond using a dragging method to make sure it has the desired orientation:

12. Continue to keep the cursor on C4.

13. Hold down the mouse button and drag upward to the right.

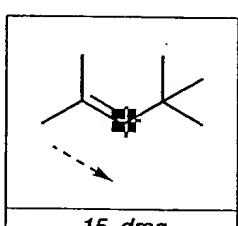
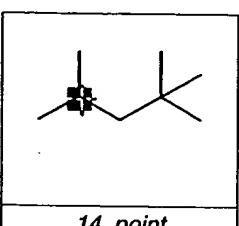
When the bond is oriented, release the mouse button to deposit the bond.



Next you will create a double bond:

14. Point to C2.

15. Drag from C2 to C3 over the existing bond to create a double bond.

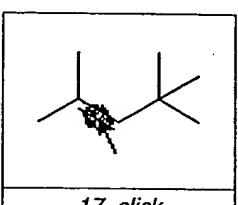
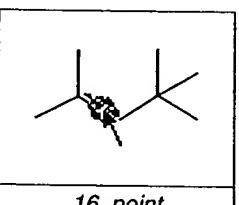


Next you will change orientation of the lines of the double bond:

16. Point to the center of the double bond.

17. Click (don't drag) to move the second bond to the outside.

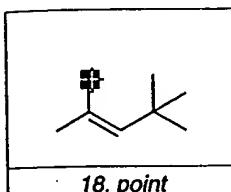
Note, you can move a double bond in this manner whenever a bond tool is the selected tool. Notice that the cursor takes on the appearance of the bond tool that is selected.



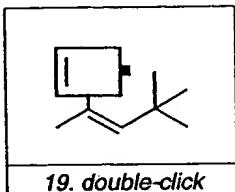
Next, you will add an atom label.

18. Point to the atom to label.

19. Double-click the atom to open a text box.

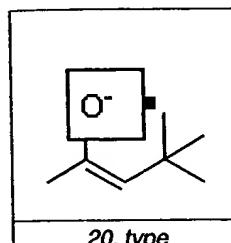


18. point



19. double-click

20. Type "O", choose superscript from the Style Submenu in the Text menu and then type "-".

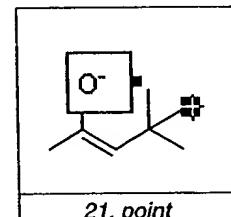


20. type

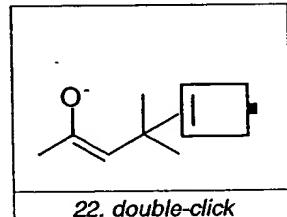
Next, you will label an atom with "OH":

21. Point to the rightmost atom.

22. Double-click the atom to open a text box.

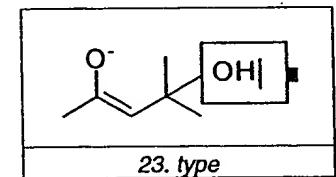


21. point



22. double-click

23..Type "OH".

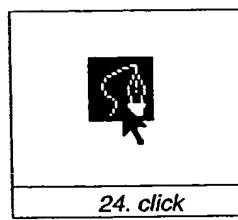


23. type

Now you need to add some arrows to indicate electron flow; however, the arrows in the arrows palette are too uniform for this purpose. Instead you can create customized arrows using the Pen tool.

24. Click the Pen tool.

25. Set the style of the curve to an arrow, by choosing Arrow at End from the Curves menu.

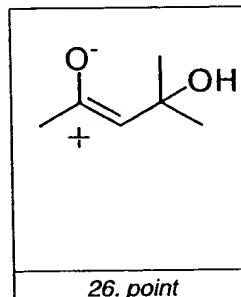


24. click

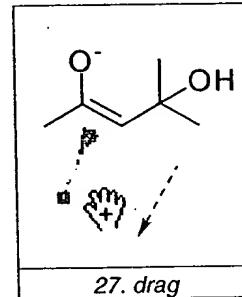
26. Point the cursor near the double bond where you want to indicate the start of electron flow.

27. Drag downwards and to the left. Release the mouse button.

The cursor changes to a hand with a "+" in it indicating that you are in the editing mode of the Pen tool.



26. point

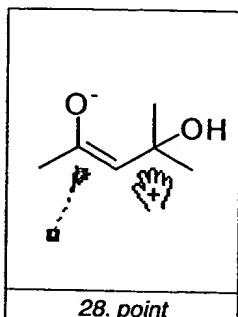


27. drag

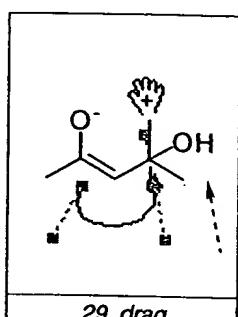
28. Position the cursor where you want the arrow head to appear.

29. Drag upwards to create a curve segment.

Press the Escape key (to exit drawing mode). The lines around the curve will then disappear.



28. point

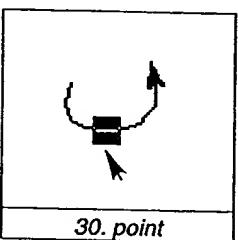


29. drag

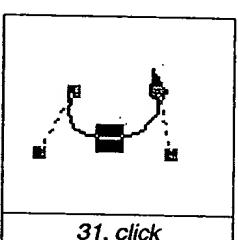
Next you will refine the shape of the arrow:

30. Point at the center of the curve until a highlight box appears.

31. Click the curve to enter edit mode.



30. point

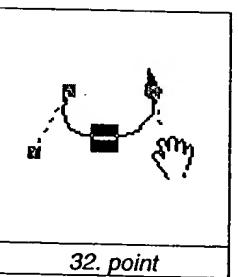


31. click

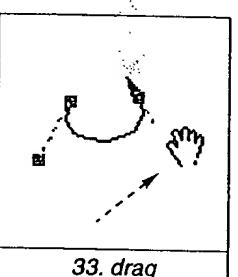
32. Point to the handle pointing away from the curve to the right (this is called a tangent handle and controls the tangent of the curve that it touches)

33. Drag the handle upwards to the left to make the arrow head point more inward.

Press the Escape key when the arrow is how you want it.

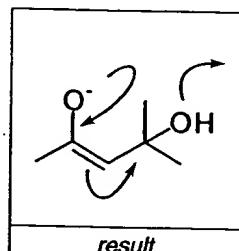


32. point



33. drag

34. Create additional arrows in the same manner and create a proton caption to complete the intermediate.

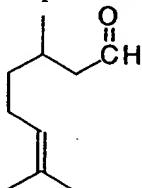


TIP: While working with arrows or other objects that are in small places, you can magnify your view using the Magnify command in the Tools menu.

- From the File menu, choose Save.
- From the File menu, choose Close.

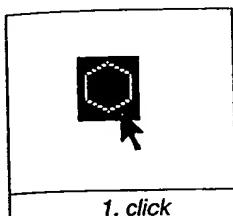
TUTORIAL 3: USING RINGS

In this tutorial you learn how to draw more complex structures by using rings:



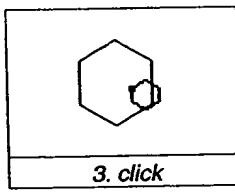
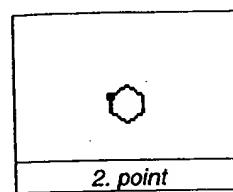
- From the File menu, choose New Document.
- From the File menu, choose Save.
- Type "tut3.cdx" in the text box.
- Select a directory (Windows) or folder (Macintosh) in which to save the file.
- Click the OK button (Windows) or the Save button (Macintosh).

1. Select the Cyclohexane Ring tool.



2. Point in an empty area of a document window.

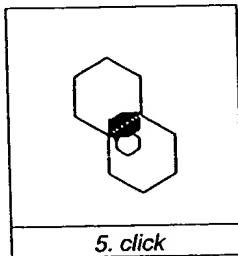
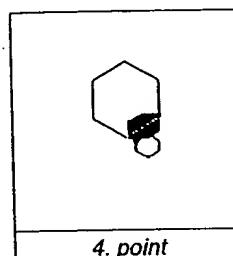
3. Click to deposit a ring.



Next, you will fuse a second ring to the first:

4. Point to the center of lower right bond in the ring.

5. Click to fuse another ring.

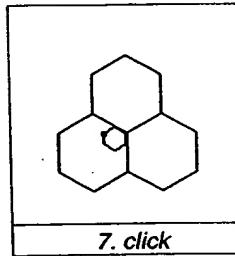
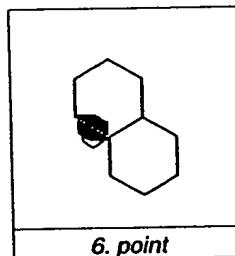


Next, you will fuse a third ring:

6. Point to the ring shown below.

7. Click to fuse another ring.

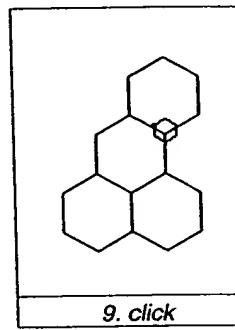
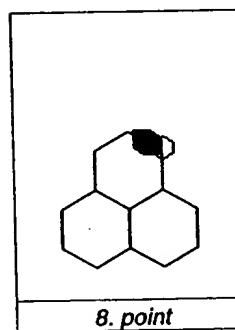
You should end up with the structure shown on the right.



Finally, you will fuse a fourth ring:

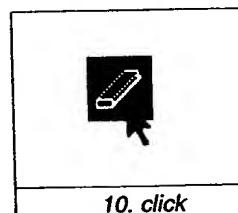
8. Point to the ring shown below.

9. Click to fuse another ring.



Next you will remove bonds in the ring using the Eraser tool.

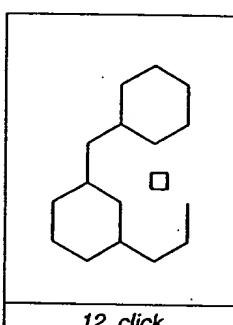
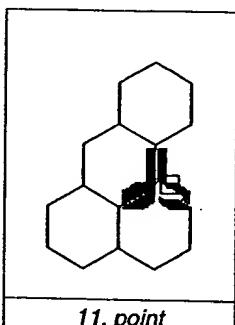
10. Select the Eraser tool.



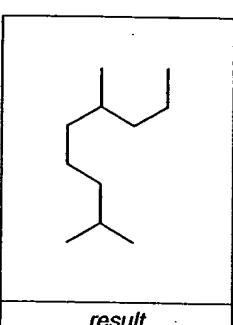
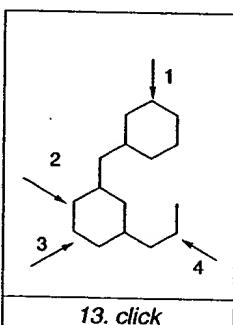
11. Point to the atom between the upper two bonds.

Highlight boxes appear on the bonds that will be removed.

12. Click to delete the atom and its bonds.

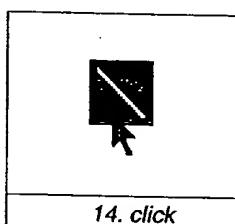


13. Continue deleting by clicking each of the atoms or bonds shown below. You should end up with the structure shown on the right.



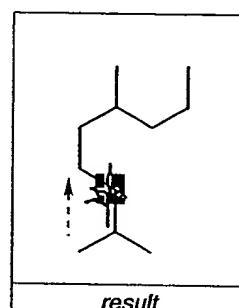
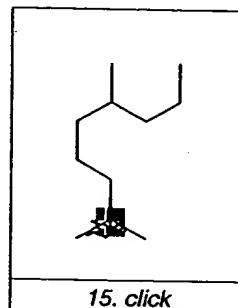
Next you will add double bonds to the structure and realign them.

14. Select the Solid Single Bond tool.



15. Point to the atom indicated below.

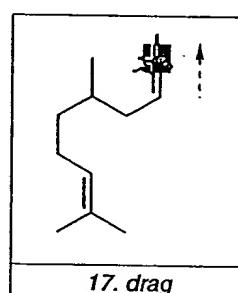
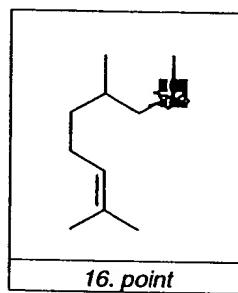
16. Drag upwards to draw a double bond.



Next, add another double bond:

16. Point to the atom indicated below

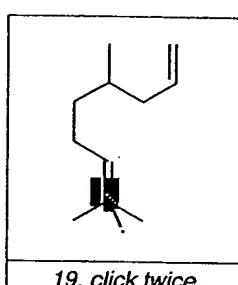
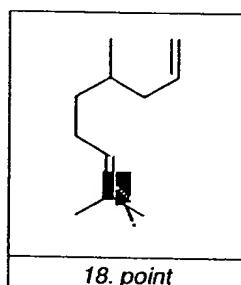
17. Drag upwards to draw a double bond.



Next you will realign the double bonds so they are centered.

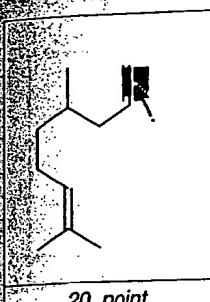
18. Point to the center of the lower double bond.

19. Click to move the line to the other side of the bond. Click again to center the bonds.

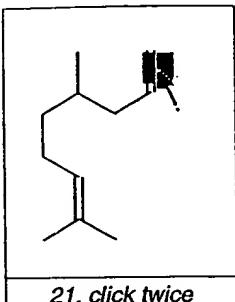


20. Point to the center of the upper double bond.

21. Click to move the line to the other side of the bond. Click again to center the bonds.



20. point



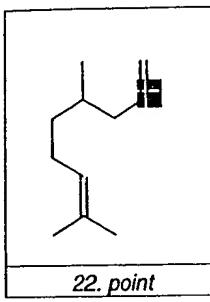
21. click twice

Next you will add a carbon atom label:

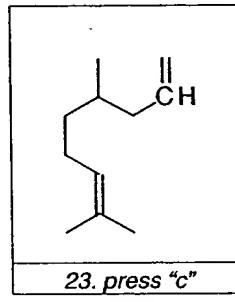
22. Point over the atom to label as carbon.

23. Press the "c" key on your keyboard. This key is a Hotkey assigned to the atom label "C".

The atom label will appear with the correct number of hydrogens.



22. point

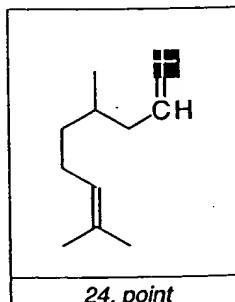


23. press "c"

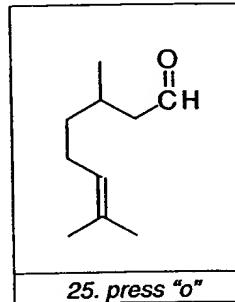
Next you will add an oxygen atom label to complete the structure:

24. Point over the atom to label as oxygen.

25. Press the "o" key on your keyboard. This key is a Hotkey assigned to the atom label "O".



24. point



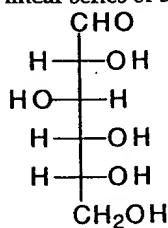
25. press "o"

- From the File menu, choose Save.

- From the File menu, choose Close.

TUTORIAL 4: FISCHER PROJECTIONS

This tutorial shows you how to draw a Fischer projection of glucose (shown below) by drawing a linear series of bonds.



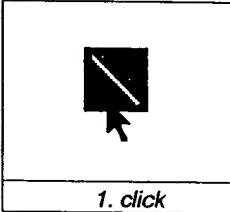
- From the Open Special submenu in the File menu choose ACS-1996.cds (Windows) or from the Windows menu choose ACS Document 1996 (Macintosh).

The new document created is based on a Style Sheet (Windows), or Stationery pad (Macintosh).

You might notice in this example that bonds and atom label fonts/sizes are different. These special documents allow you to have pre-configured settings for different tasks. In this example, the ACS template is used to help maintain information for a one-column layout (a Page Setting), for bonds with a Fixed length of 0.2 inches (a Drawing Setting), and for Atom Labels in Times Font (a Text Setting). This is the desired setting for structures to be published in all ACS journals.

- From the File menu, choose Save As.
- Select a directory (Windows) or folder (Macintosh) in which to save the file.
- Type "tut4.cdx" in the text box at the bottom of the Save dialog box.
- Click the OK button (Windows) or Save button (Macintosh).

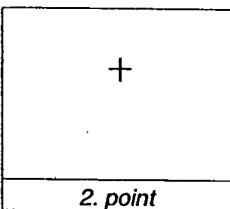
1. Select the Solid Bond tool.



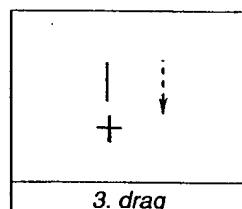
1. click

2. Point in the document window.

- 3. Hold down the mouse button and drag vertically to draw your first bond.



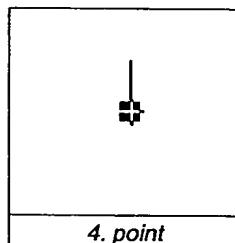
2. point



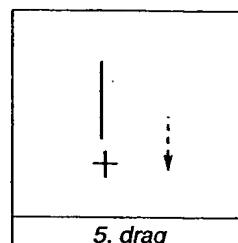
3. drag

Next, add another bond:

4. Point to the lower atom.
5. Hold down the mouse button and drag downward to draw the second bond.



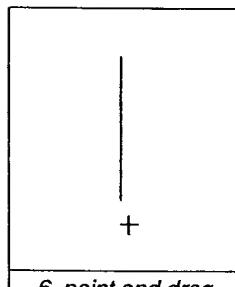
4. point



5. drag

6. Repeat above step 4 and 5 three more times for a total of five bonds.

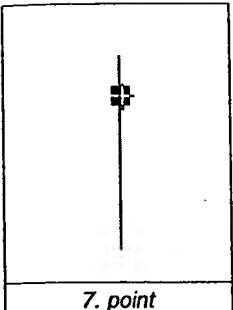
NOTE: Drag the pointer along the length of the bonds you drew, you will see the pointer alternate between an arrow and a cross. The arrow indicates you are pointing over the center of a bond, and the cross indicates you are pointing to an atom.



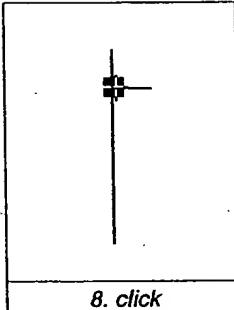
6. point and drag
three more times

Next, you will add a horizontal bond to the second atom in the string of bonds you created:

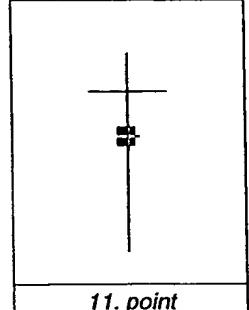
7. Point to C2.
8. Click the atom to add a perpendicular bond.



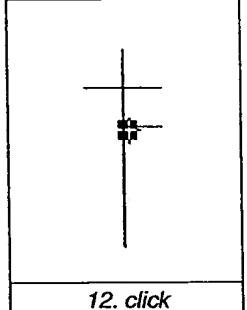
7. point



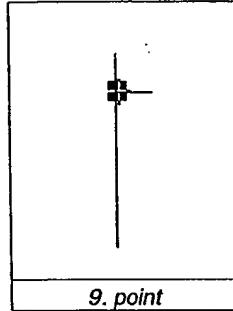
8. click



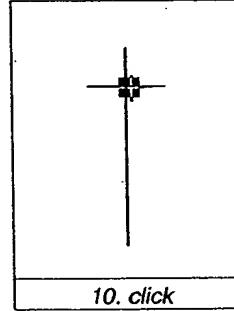
11. point



12. click



9. point

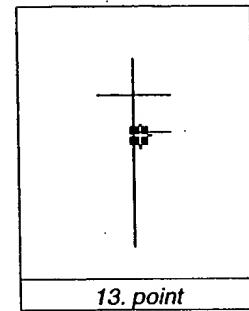


10. click

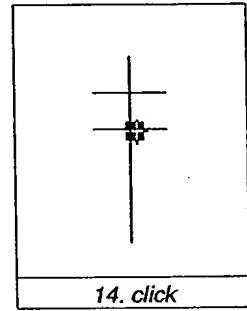
Next you will add a bond to the next atom in the line of bonds.

11. Point at the third atom (C3).

12. Click the atom to add a perpendicular bond.

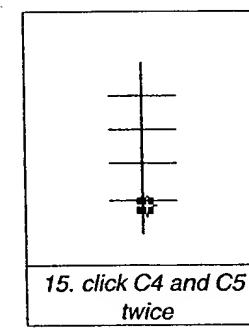


13. point



14. click

15. Repeat steps 13 and 14 for the for the fourth (C4) and fifth (C5) atoms.

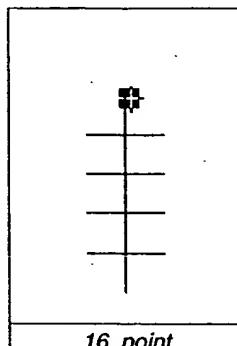


15. click C4 and C5 twice

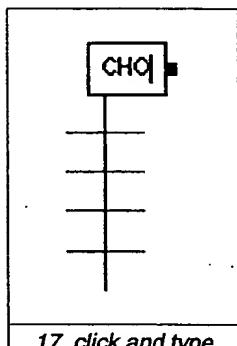
Next, add a label to C1:

16. Point to C1.

17. Double-click C1 to create a text box, then type CHO.



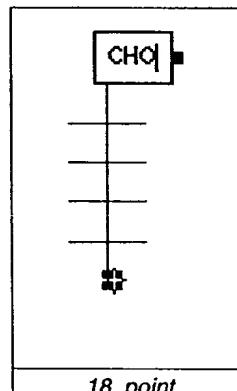
16. point



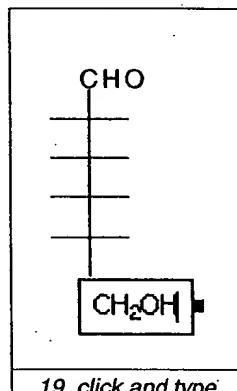
17. click and type

18. Point to C6.

19. Double-click C6 to create a text box, then type CH₂OH. Click outside the text box to close it.



18. point

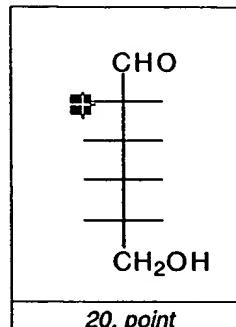


19. click and type

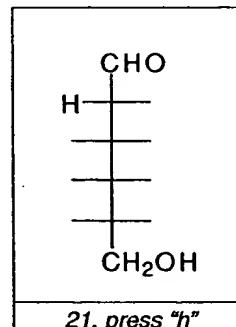
Next add the H, and OH labels:

20. Point to the atom shown below.

21. Press the key "h" to label the atom with a Hydrogen.

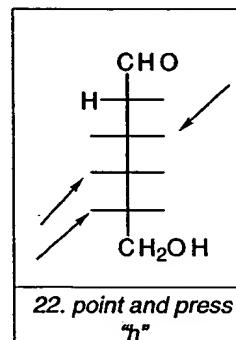


20. point

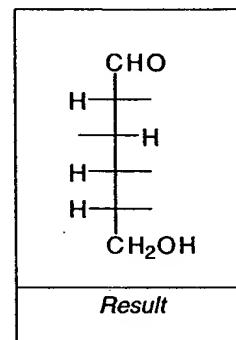


21. press "h"

22. Repeat this labeling procedure for the remaining atoms that are hydrogen indicated by arrows below on the left.



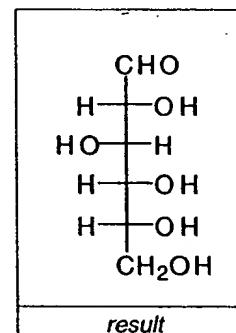
22. point and press "h"



Result

Next, label the OH's:

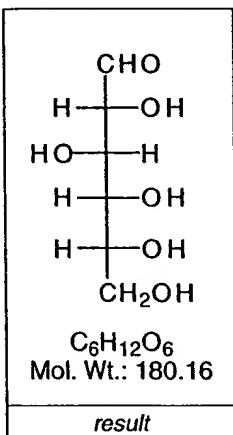
23. Repeat this labeling procedure for the remaining atoms pressing the Hotkey "o" to label them with OH. The result should appear as shown below.



result

As a final step, you will check the chemical syntax of the structure you drew followed by automatically calculating the formula and molecular weight.

24. Select the Selection tool to automatically select the last structure drawn. If the structure is not selected for whatever reason, double-click the structure.
25. From the Object menu, choose Analyze Structure. If drawn correctly, a dialog box with information calculated from the structure appears (if errors are present, a check structure message appears indicating the problem).
26. In the dialog box that appears, deselect all but the Formula and Molecular Weight checkboxes.
27. Click the Paste button to paste the information as a caption below the structure.
28. Click outside the caption to deselect it.



- From the File menu, choose Save.
- From the File menu, choose Close.

TUTORIAL 5: PERSPECTIVE DRAWINGS

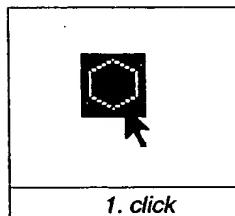
In this exercise you will learn how to create perspective drawings by drawing D-glucose as a Haworth projection.

- From the File menu, choose New.

NOTE: The new command will be appended with the last stationery pad/style sheet used. If you are working from tutorial 4, the name of the command will be New ACS-1996 (Windows) or New ACS Document 1996 (Macintosh).

- From the File menu, choose Save.
- Select a directory (Windows) or folder (Macintosh) in which to save the file.
- Type "tut5.cdx" in the text box at the bottom of the dialog box.
- Click the OK button (Windows) or the Save button (Macintosh).

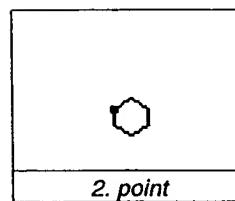
1. Select the Cyclohexane ring tool.



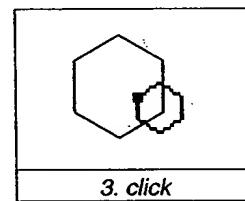
1. click

2. Point in an empty area of a document window.

3. Click to deposit a ring.

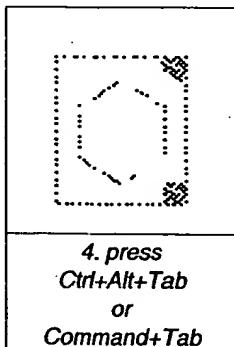


2. point



3. click

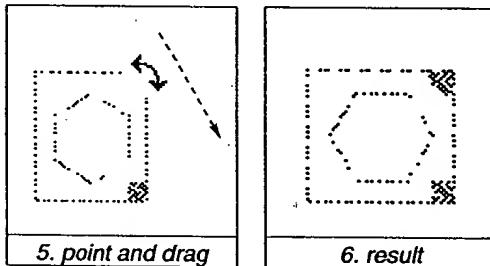
4. Press Ctrl+ Alt+Tab keys (Windows) or Command+Tab key (Macintosh) to automatically select the Selection tool and the last structure drawn.



5. Point to the upper right corner of the Selection Rectangle (the Rotation handle).

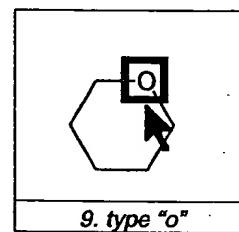
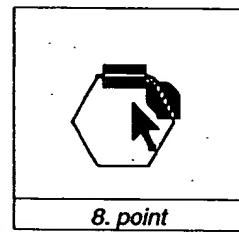
NOTE: The cursor changes to a curved double-sided arrow indicating the rotation mode of the Selection tool is activated.

6. Drag the Rotation handle to the right about 30 degrees (look at the Messages area at the lower left of the window).



NOTE: Even though you have fixed angles on, the angle is not constrained. Fixed angles only applies when you are drawing with the tool used to create it. For example, if you had created this ring by dragging rather than clicking, the angle you could use would be constrained if Fixed Angles is on. Try it out!

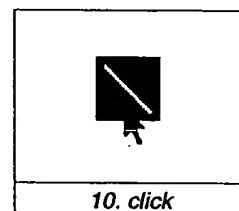
7. Click outside the structure to deselect it.
8. Point to the atom indicated below on the left.
9. Press the HotKey "o".



NOTE: When you are using the Selection tool, the bonds attached to the atom you are pointing at are highlighted. If you were to click, you would select these bonds. However, when you use a HotKey while using the Selection tool, the atom is labeled. Also note that the shape of the highlight boxes differs depending on whether you are working on a Macintosh or Windows computer - the picture above is from a Macintosh.

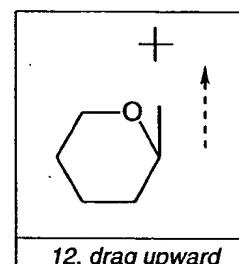
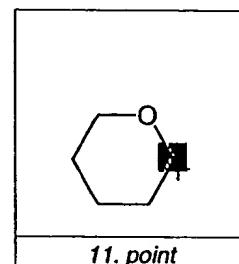
Next, add vertical bonds:

10. Click the Single Bond tool to select it.



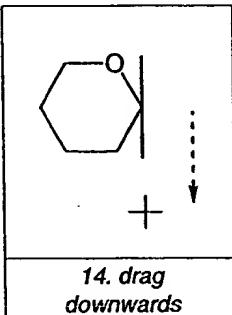
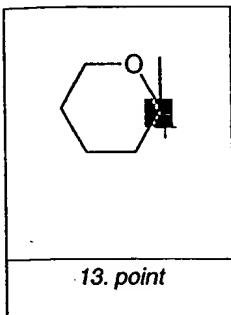
11. Point to C1 (to the right of the oxygen)

12. Drag upwards to create a bond.

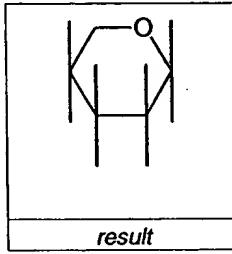
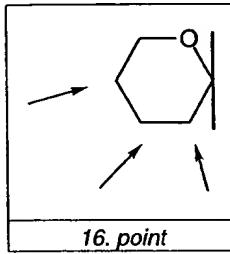


13. Point to C1 again

14. Drag downwards to create another bond.



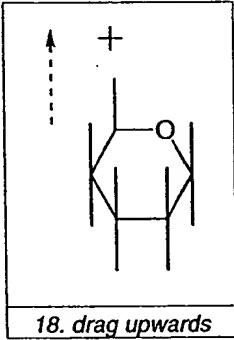
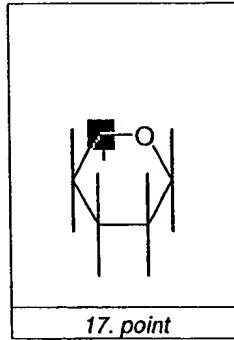
15. Repeat for C2 through C4 as indicated by the arrows in the lower left illustration. The result will appear as the right illustration.



Next, draw one upwards bond at C5:

17. Point to C5.

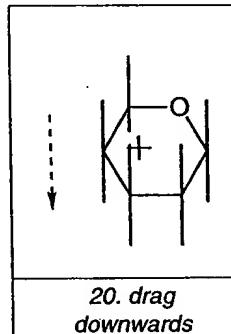
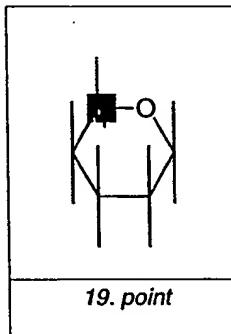
18. Hold down the mouse button and drag upwards.



For the downward bond for C5, you will need to turn Fixed lengths off. Otherwise, the bond will be joined to the upward bond of C3. You can temporarily disable Fixed lengths using a modifier key.

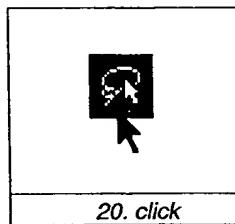
19. Point to C5.

20. Hold down the Alt key (Windows) or Command key (Macintosh), then hold down the mouse button and drag downward from C5. Stop dragging about half the distance to the upward bond on C3.



Next you will distort the structure to change its aspect ratio. This will give the perspective of viewing the structure along the Z-axis.

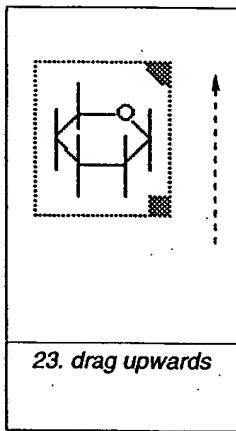
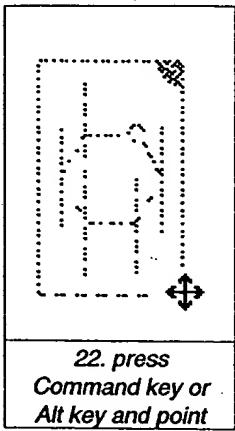
21. Select the Selection tool by clicking its icon.



22. Point to the Resize handle(lower right corner) and hold down the Alt key (Windows) or the Command key (Macintosh).

NOTE: The cursor changes to a cross with arrows at each end indicating the distortion function of the Selection tool is activated.

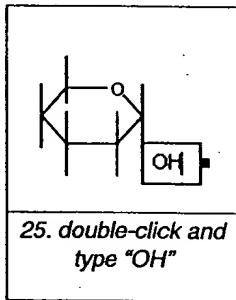
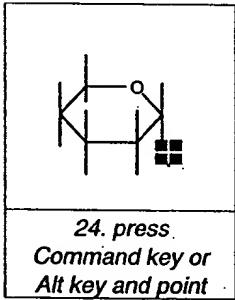
23. Drag upwards until you have distorted the structure to about 50% (shown in the Messages area of the window).



Next you will create OH labels. Since this label is repeatedly used, you will learn how to repeat a label. Only labels where you have opened a text box will be repeatable.

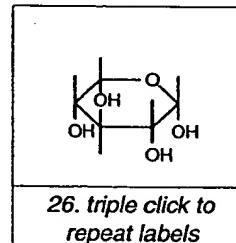
24. Select the single bond tool, point to the atom shown on the left and double-click to open a text box.

25. Type OH, and move the pointer to the next atom as shown and triple-click to repeat the atom label.



26. Triple-click the remaining atoms (as shown below) to repeat the OH label.

NOTE: You can choose the Magnify command from the tools menu if you find it difficult to place the labels.

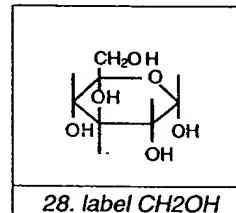


Next, add the CH₂OH label:

27. Triple click the upper atom of C5.

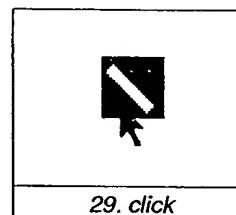
28. Next, press the Return key to open the atom label text box and type CH₂ before the OH.

NOTE: This last step showed you another HotKey, namely the "Return" key, that opens a text box for the last atom labeled. The definition for this particular HotKey cannot be changed.



In this final step you will change the type of the frontmost bonds.

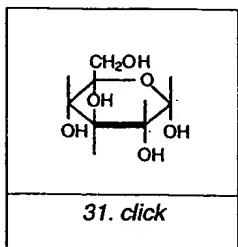
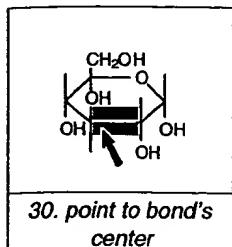
29. Click the bold bond tool.



29. click

30. Point to the center of the frontmost bond

31. Click to change to the new bond type.



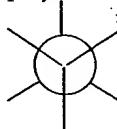
NOTE: If the highlight box disappears, you have moved the pointer too far. You may want to magnify your view using the Magnify command in the Tools menu if you find it difficult to place the pointer where you want.

NOTE: If the wedge is pointed in the wrong direction, click the bond again to flip its orientation.

- From the File menu, choose Save.
- From the File menu, choose Close.

TUTORIAL 6: NEWMAN PROJECTIONS

This tutorial shows you how to draw a Newman projection.

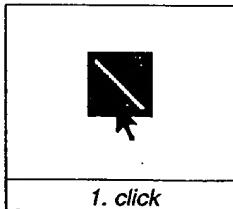


- From the File menu, choose New.

NOTE: This command will read "New ACS Document 1996" if you just completed the last tutorial.

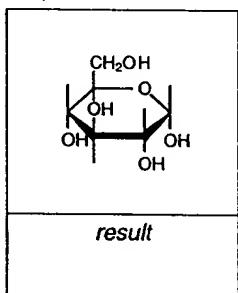
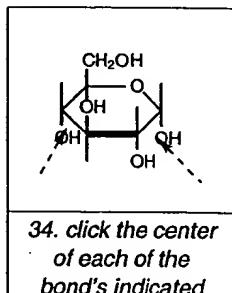
- From the File menu, choose Save As.
- Select a directory (Windows) or folder (Macintosh) in which to save the file.
- Type "tut6.cdx" in the text box and click the Save button (Macintosh) or OK button (Windows).

1. Click the Solid Bond tool to select it.

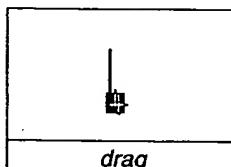
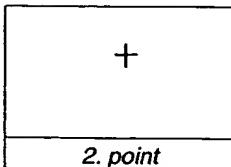


33. Point to the bond to the right of the bond you changed.

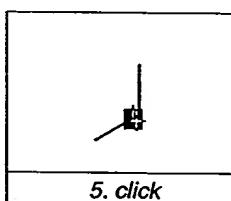
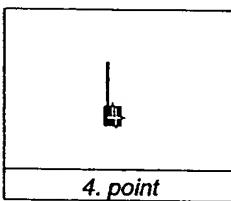
34. Click slightly off center in the direction that you want the wide end of the wedge to be oriented, then click.



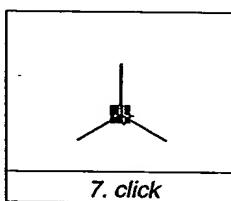
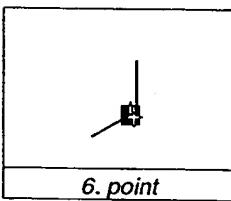
2. Point in the document window.
3. Drag downwards to create the first bond.



4. Continue pointing at the lower atom.
5. Click again to add a second bond.

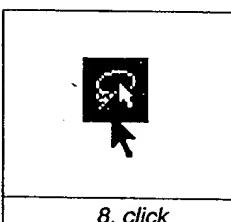


6. Continue pointing at the same atom
7. Click again to add a third bond.



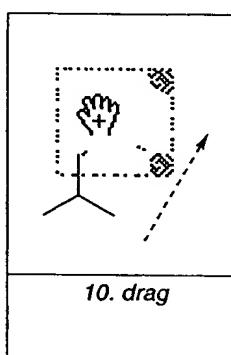
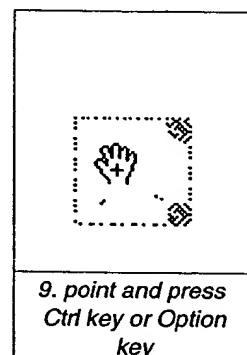
8. Select the Selection tool by clicking its icon.

The last structure you drew is automatically selected.



9. Point within the Selection rectangle. Hold down the Ctrl key (Windows) or Option key (Macintosh).

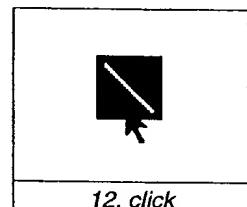
10. Hold down the mouse button and drag a copy of the structure diagonally upward to the right of the original.



11. Release the mouse button (and depressed key) when the copy is positioned.

Next you will add a bond between the duplicated structures:

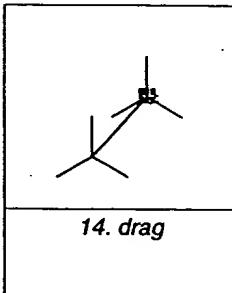
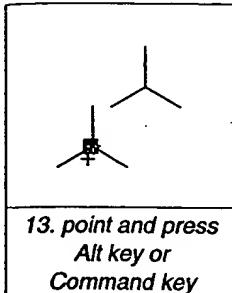
12. Click the Solid Bond tool to select it..



13. Point to the central atom of the lower fragment. Hold down the Alt key (Windows) or Command key (Macintosh).

14. Hold down the mouse button and drag to the central atom of the upper fragment.

Release the mouse button when the highlight box over the central atom appears.

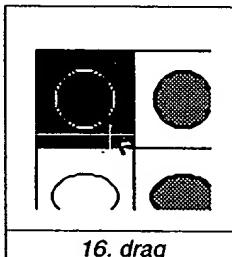
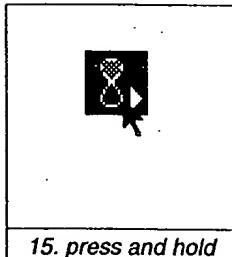


NOTE: The modifier key used in this step removes the fixed length constraint so you can draw a longer bond that will reach the upper fragment. Fixed angles are also disabled.

This example is not using an orbital as an orbital. Instead, you will use the Orbital tool to draw the hollow circle that is particular to Newman Projections.

15. Hold down the mouse button over the Orbital tool to display its palette.

16. Drag to the unfilled s orbital (first column, first row).

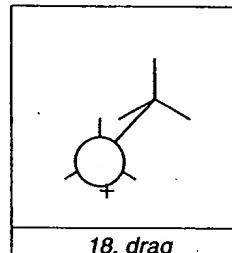
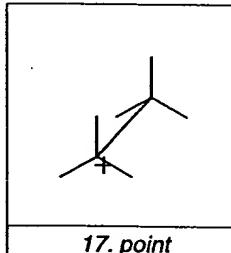


17. Point to the left center carbon, hold down the Alt key (Windows) or Command key (Macintosh).

18. Hold down the mouse button and drag outward. Notice that a highlight box doesn't appear over the atom. The orbital tool does not change as if you were adding bonds or atoms to the structures. Thus, you may want to group the orbital with the structure to make it moveable as a unit.

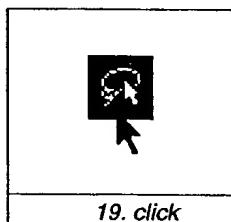
NOTE: The size of the orbital is constrained just like bonds. The constraint is based on a percentage of the Fixed length setting in the Drawing Settings dialog box.

NOTE: Whenever you want to add orbitals to a structure, you drag starting from the atom that you want to position the center or node.



Next you will move part of the structure to the front so overlap the orbital:

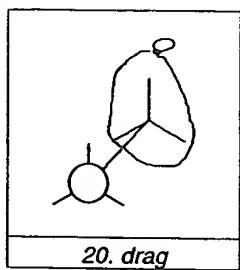
19. Click the Selection tool.



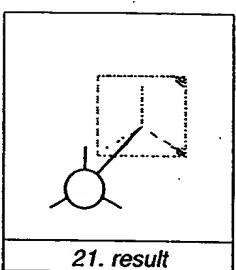
20. Point above the structure

21. Hold down the mouse button and drag around the upper fragment to select the three bonds

NOTE: This is another example of the default mode of the Selection tool called the Lasso. Only bonds that are completely within the Lasso area are selected. You don't want the bond connecting the two fragments to be selected. If you find this difficult to do with the lasso, you may wish to Shift+click on each bond separately.



20. drag

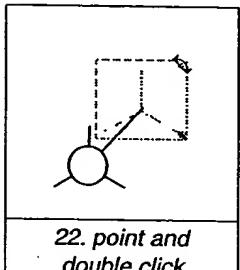


21. result

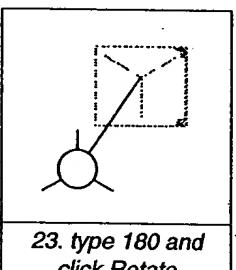
Next, you will rotate the selection:

22. Double-click the Rotation handle in the upper right of the Selection Rectangle to open the Rotate dialog box.

23. Type 180 in the text box and click the Rotate button.



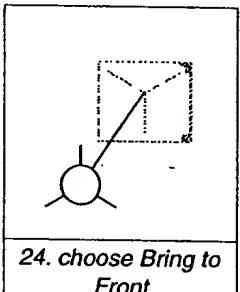
22. point and double click



23. type 180 and click Rotate

Next, you will change the layering of the structure so that the selection is frontmost.

24. From the Object menu, choose Bring to Front.

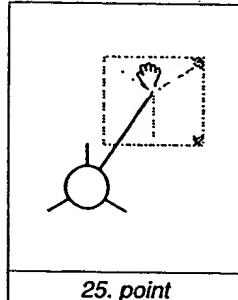


24. choose Bring to Front

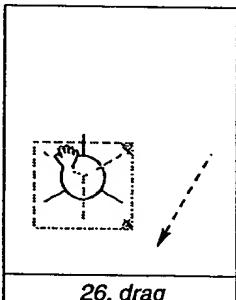
Finally, you will orient the frontmost part of the structure to create a Newman projection.

25. Point within the Selection Rectangle until the pointer changes to a hand.

26. Drag the selection until the central atom of the selection is centered within the orbital. Release the mouse button and click outside the Selection Rectangle to deselect the structure.



25. point



26. drag

- From the File menu, choose Save.

- From the File menu, choose Close.

Chapter 3, Drawing Chemical Structures

At the heart of *ChemDraw* are tools specially designed for drawing chemical structures: nine bond tools, ten ring tools, and an acyclic chain tool. This chapter describes how to create chemical structure drawings using these tools.

SINGLE BONDS

Nine bond tool icons are located in the Tools palette. The icons representing each tool are shown below (Table 3-1):

Table 3-1 Single bond tool icons



Solid Bond



Dashed Bond



Hashed Wedged Bond



Bold Wedged Bond



Hashed Bond



Bold Bond



Hollow Wedged Bond



Wavy Bond



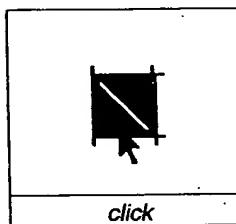
Dative Bond

Selecting a Bond Tool

To select a bond tool:

- Click a bond tool icon in the Tools palette.

Figure 3-1 Selecting a bond tool



Drawing Bonds

You can draw bonds that are either constrained to a fixed length or have variable lengths. You can also draw bonds with a fixed or variable angle relative to the X axis.

Fixed Lengths

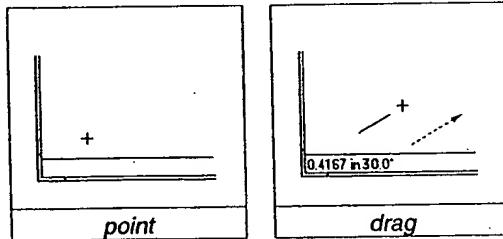
To draw bonds that are constrained to a fixed length:

- From the Tools menu, choose Fixed Lengths.

A check mark appears next to the Fixed Lengths command indicating that it is turned on. When Fixed Lengths is turned on, all the bonds drawn are constrained to the fixed length specified in the Drawing Settings dialog box.

- Select a bond tool.
- Drag from one end of the bond to the other.

Figure 3-2 Drawing the first bond



The Message area at the bottom left of a document window shows the length and angle of the bond as you drag. The bond will not extend further than the fixed length. Also see "Message Area" later in this chapter for further information.

Drawing Settings Guide

Fixed Length

Bonds drawn when Fixed Length in the Tools menu is turned on are constrained to the value set in the Fixed Length box in the Drawing Settings dialog box.

To change the Fixed Length value:

- Choose Drawing Settings from the File menu.
- Type a value in the Fixed Length text box and click the OK button.

This change affects the current document only. See "Saving Customized Settings" in Chapter 1, *ChemDraw Basics* to learn how to make the change permanent.

Fixed Angles

To draw bonds that are constrained to angles that are multiples of 15 degrees relative to the X axis:

- From the Tools menu, choose Fixed Angles.

A check mark appears next to the Fixed Angles command indicating that it is on.

- Select a bond tool by clicking its icon.
- Drag from one end of the bond to the other in a document window.

The Message area indicates that the bond angle is constrained to 15 degree increments. Also see "Message Area" later in this chapter.

Drawing Unconstrained Bonds

To draw a bond that is not constrained to a fixed length or fixed angle:

- From the Tools menu, choose Fixed Lengths and Fixed Angles if they are presently checked.

The absence of a check mark next to the Fixed Lengths or Fixed Angles command in the Tools menu indicates the commands are off.

- Select a bond tool by clicking its icon.
- Drag from one end of the bond to the other in a document window.

You can draw any bond length and create any angle relative to the X axis. The Message area displays the length of the bond and the angle it makes with the X axis as you drag the bond.

Shortcut - Toggling Fixed Length and Fixed Angle

To temporarily toggle Fixed Lengths and Fixed Angles on and off:

- Alt+drag (Windows) or Command+drag (Macintosh) from one end of a bond to the other end in the document window.

If Fixed Lengths or Fixed Angles are turned on, you can hold down the Alt key (Windows) or the Command key (Macintosh) to temporarily turn off these constraints.

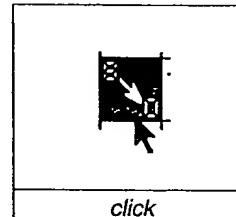
Dative Bonds and Wedged Bonds

Dative bonds and wedged bonds are drawn with a specific orientation in a document window.

To draw a dative bond:

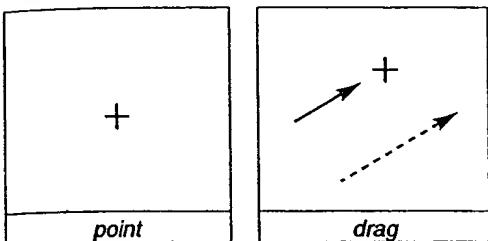
- Select the Dative Bond tool.

Figure 3-3 Dative bond tool



- Drag from the positive to the negative end (arrow head) of the dative bond.

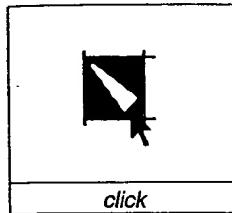
Figure 3-4 Drawing a dative bond



To draw a wedged bond:

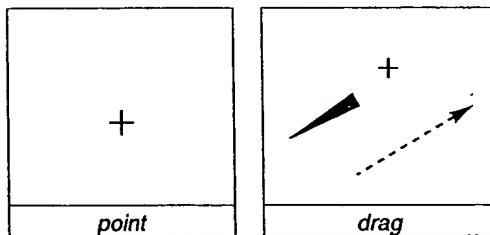
- Select one of the wedged bond tools.

Figure 3-5 Wedged bond tool



- Drag from the narrow end of the wedged bond to the wide end of the wedged bond.

Figure 3-6 Drawing a wedged bond



If the orientation of the dative bond is not what you want:

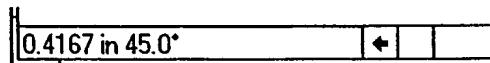
- Click the center of the dative or wedge bond using its tool.

The orientation of the bond is inverted.

Message Area

As you draw bonds, information appears in the Message area at the lower left corner of a document window. The message area in Figure 3-7 shows the bond length and angle the bond makes with the x-axis

Figure 3-7 Message area



The number on the left indicates the length of the bond you are drawing. The number on the right indicates the counterclockwise angle between the bond and the positive X axis.

Preferences Guide

Units

The units used in the Rulers, Crosshair and Drawing Settings can be set to centimeters, inches, or points.

To change the units:

- From the File menu, choose Preferences.
- Choose a unit measurement from the Units pop-up menu, then click the OK button.

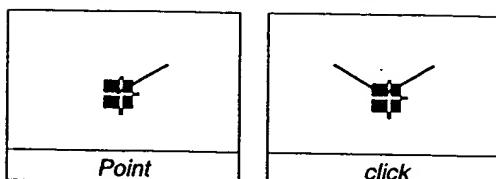
This change affects all documents.

Adding a Bond by Clicking

To quickly add a fixed length bond:

- Select a bond tool by clicking its icon.
- Click an atom.

Figure 3-8 Adding a bond by clicking



A new bond is drawn and is joined to the atom you clicked. Bonds drawn by this method are always drawn using the Fixed Length specified in the Drawing Settings dialog box. The angle that the deposited bond makes with its nearest neighbor is equal to the Chain Angle set in the Drawing Settings dialog box. If this angle cannot be established, a smaller angle is used.

Adding Bonds by Dragging

To control the orientation of bonds that you draw, you can add bonds by dragging

- Select a bond tool.
- Point to an atom.

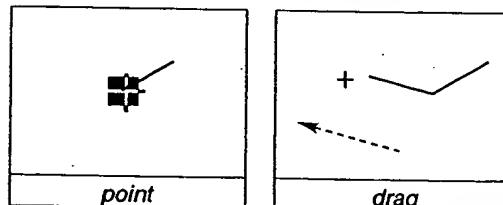
A highlight box appears over the atom indicating where the bond will be joined (if you are pointing to a bond, the highlight box encompasses the entire bond).

- Drag from the atom at which you are pointing to the end of the new bond.

If Fixed Lengths is turned on, the length of the bond will be constrained. If Fixed Angles is turned on the angle will be constrained to 15 degree increments.

A new bond is drawn and joined to the atom where the highlight box appeared. By using this dragging method for drawing the bond, you can control the orientation of the other end of the bond.

Figure 3-9 Adding a bond by dragging



Preferences Guide

Tolerance

The size of highlight box is controlled by the value in the box labeled "Tolerance" in the Preferences dialog box. The default setting for the Tolerance is 5 pixels. This means, for instance, that the highlight box appears on atoms if the pointer is located in a square region 10 pixels on a side or +/- 5 pixels from the atom.

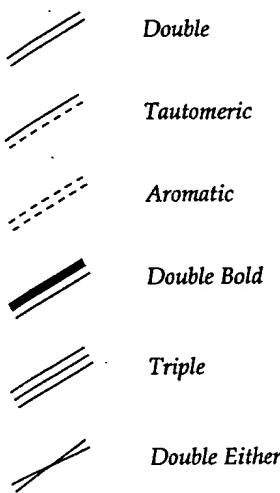
To change the Tolerance:

- From the File menu, choose Preferences.
- Click the up or down Tolerance control arrow to increase or decrease the tolerance, then click the OK button.

MULTIPLE BONDS

You can use the Solid, Dashed, and Bold Bond tools to create the following multiple bonds:

Table 3-2 Types of multiple bonds



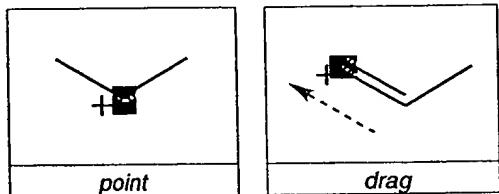
Double Bonds

To draw a double bond:

- Select the Solid, Dashed or Bold bond tool.
- Drag over an existing bond from one end of the bond to the other end.

A double bond is created.

Figure 3-10 Drawing a double bond



Double Either Bonds

To create a double either bond:

- Draw a double bond using the Solid Single bond tool.
- Select the Wavy bond tool.
- Point to the center of the double bond and click.

Triple Bonds

You can draw a triple bond by drawing another single bond on top of a double bond.

To draw a triple bond:

- Select any bond tool.
- Drag from one end of an existing double bond to the other.

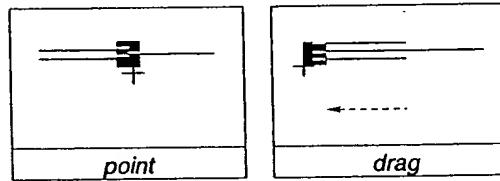
All bonds in a triple bond are solid bonds.

To change a triple bond into a single bond:

- Select any bond tool.
- Drag from one end of an existing triple bond to the other.

The triple bond changes into a single bond that corresponds to the tool you used to draw over the bond. Another way to reduce the bond order is to use the Eraser tool. See “Eraser Tool” in *Chapter 7, Working with Selections*.

Figure 3-11 Drawing a triple bond



RING TOOLS

There are ten ring tools available for drawing various ring sizes and types:

Table 3-3 Available ring tools



Cyclopropane Ring Tool



Cyclobutane Ring Tool



Cyclopentane Ring Tool



Cyclohexane Ring Tool



Cycloheptane Ring Tool



Cyclooctane Ring Tool



Cyclohexane Chair Ring Tool (1)



Cyclohexane Chair Ring Tool (2)



Cyclopentadiene Ring Tool



Benzene Ring Tool

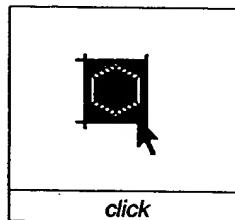
NOTE: (Macintosh only) If you are using a small monitor, such as found on the Macintosh SE/30, several of the Cycloalkane Ring tools are grouped into a pop-up palette.

Selecting a Ring Tool

To select a Ring tool:

- Click a Ring Tool icon in the Tools palette.

Figure 3-12 Selecting the cyclohexane ring tool



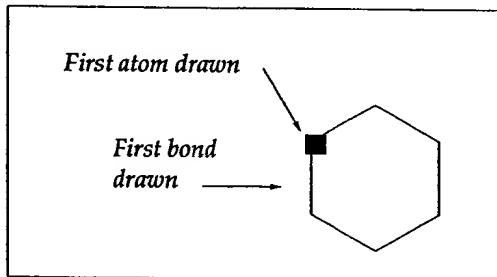
Drawing a Ring

To draw a ring:

- Select a Ring tool.
- Position the pointer in a document window.

When you point in a document window, the pointer changes to a ring tool pointer (as shown in Figure 3-13). The highlight box on the ring tool pointer indicates the atom that is drawn first. The bond directly below the highlight box is the bond that is drawn first.

Figure 3-13 Ring tool cursor (enlarged)



- Drag from the beginning to the end of the first bond.

If Fixed Lengths is on when you draw a ring, the length of each bond in the ring is automatically set to the fixed length. If Fixed Angles is on, the angle the first bond in the ring makes with the X axis is restricted to 15 degree increments. See "Drawing Bonds with Fixed Lengths and Fixed Angles" earlier in this chapter for more information.

Figure 3-14 Drawing a cyclohexane ring

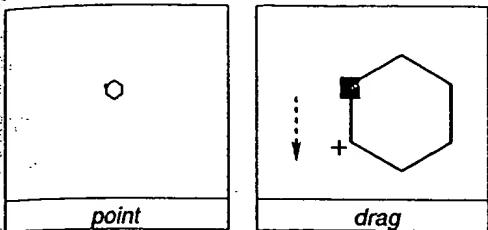
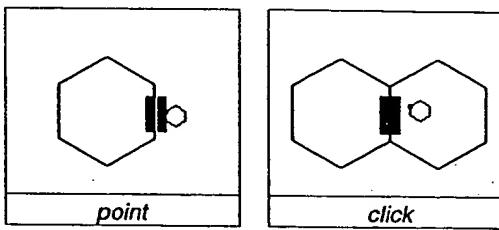


Figure 3-16 Fusing a cyclohexane ring



Depositing a Ring by Clicking

To quickly draw a ring:

- Select a Ring tool and click In a document window.

A ring appears in a document window centered around the pointer. The ring is drawn using the Fixed Length specified in the Drawing Settings dialog box. The ring is deposited in the orientation shown on the ring tool icon.

If you click a bond, the ring is fused to that bond. If you click an atom, the ring is attached to that atom, if the atom is in a ring, a spiro-linkage is formed. If you click in an empty area in the document window, the ring is centered around that point.

Figure 3-15 Adding a cyclohexane ring

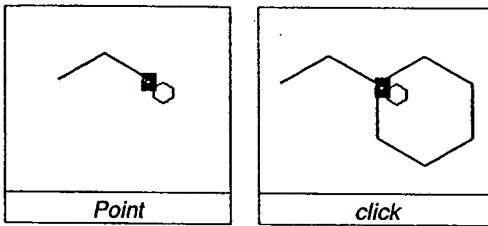
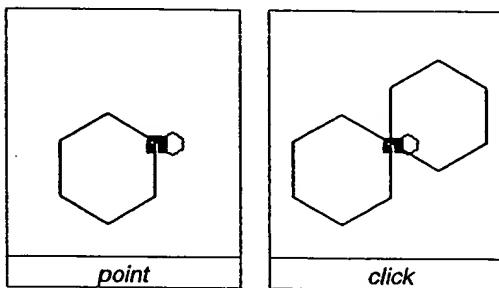


Figure 3-17 Creating a spiro linkage



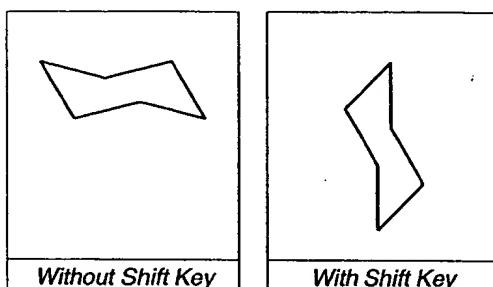
Cyclohexane Chair Ring Tools

The cyclohexane chair ring tools can be drawn in two orientations (Figure 3-18). Using the methods previously discussed, the chair is drawn in a horizontal orientation.

To change a cyclohexane chair ring to a vertical orientation:

- Select one of the Cyclohexane Chair Ring tools.
- Shift+drag from the beginning of the first bond to the end of the bond or, Shift+click in a document window.

Figure 3-18 Shift key effect on cyclohexane chair rings orientation



Resonance Delocalized Rings

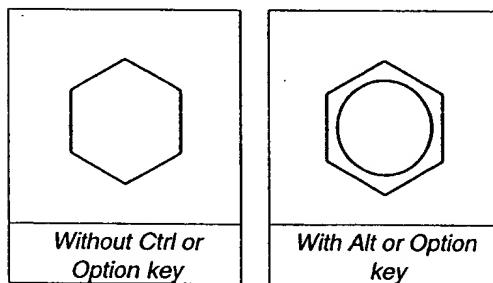
Any of the ring tools, except the cyclohexane chairs, can be drawn in a resonance delocalized form.

To draw a resonance delocalized ring:

- Select a Ring tool.
- Hold down the Ctrl key (Windows) or the Option key (Macintosh) and drag or click to draw the ring.

A circle appears inside the ring.

Figure 3-19 Option key effect on ring tool drawing



NOTE: The circle is automatically grouped with the ring when drawn. For a discussion of grouping objects, see "Grouping" in Chapter 7, Working with Selections.

Cyclopentadiene and Benzene Ring Tools

The double bonds in the cyclopentadiene or benzene ring tools can be drawn in either of two orientations.

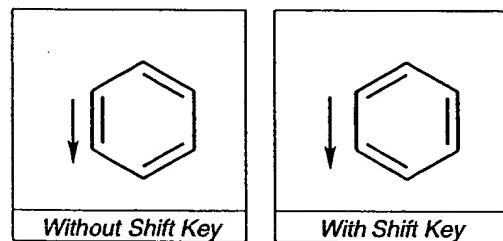
Normally, the first bond drawn is a double bond. This is the orientation indicated on the cyclopentadiene and benzene ring tool pointer. You can draw in this orientation by the methods previously discussed.

To shift the orientation so that the first bond drawn is a single bond:

- Shift+drag from the beginning of the first single bond to the end of the single bond.
- Or, Shift-click in a document window to deposit the bond with a Fixed Length.

In Figure 3-20, the arrow indicates the direction the first bond is drawn.

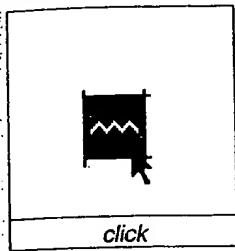
Figure 3-20 Shift key effect on benzene right orientation



ACYCLIC CHAINS

Using the Acyclic Chain tool, you can draw long hydrocarbon chains.

Figure 3-21 The Acyclic chain tool



Selecting the Acyclic Chain Tool

To select the Acyclic Chain tool:

- Click the Acyclic Chain Tool icon in the Tools palette.

Drawing an Acyclic Chain

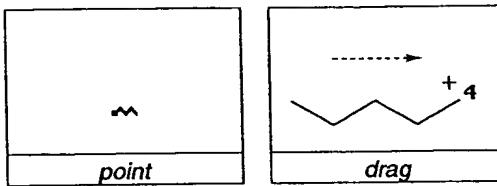
To draw an acyclic chain:

- Click the Acyclic chain tool to select it.
- Drag in the direction you want the chain to grow in a document window.

A number appears at the end of the chain indicating how many bonds you have drawn.

When Fixed Lengths is on, the pointer on the acyclic chain can be dragged to make any angle relative to the X axis. At a constant chain length, the position of the first bond, and all subsequent odd-numbered atoms will depend on the direction you drag. Before releasing the mouse button, this position can be changed by dragging in the opposite direction. When Fixed Angles is on, the angle the acyclic chain can make relative to the X axis is constrained to 15 degree increments. The internal angle between the bonds of the chain is specified by the Chain Angle spin button in the Drawing Settings dialog box.

Figure 3-22 Drawing a chain by dragging

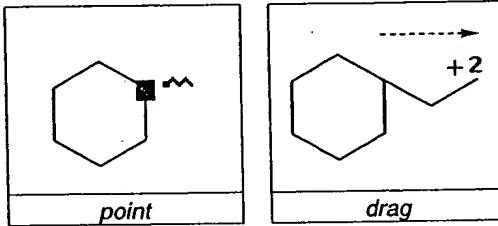


Adding Chains

To add an Acyclic Chain to an existing atom:

- Select the Acyclic Chain tool.
- Point to the atom to which you want to attach the chain.
- Drag in the direction you want the chain to grow.

Figure 3-23 Adding a chain to an existing atom

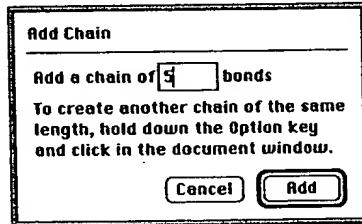


To specify a chain length:

- Select the Acyclic Chain tool.
- Click an existing atom or an empty area in a document window.

The Add Chain dialog box appears.

Figure 3-24 Add Chain dialog box



- Type the number of bonds in the chain.
- Click the Add button.

To add another chain of the same length anywhere in a document window:

- **Ctrl+click (or Option+click) an existing atom or click in an empty area within the document window.**

Drawing Settings Guide

Chain Angle

All of the bond angles in an acyclic chain are equal. The size of this angle is controlled by the Chain Angle value in the Drawing Settings dialog box. The angle is measured in degrees. You can set the angle at any integral value between 1° and 179° degrees.

To change the chain angle:

- Select Drawing Settings from the File menu.
- Click the up or down Chain Angle control arrow to increase or decrease the angle.
- Click the OK button.

This change affects the current document only. See "Saving Customized Settings" in *Chapter 1, ChemDraw Basics* to learn how to make the change permanent.

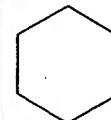
DRAWING SETTINGS FOR BONDS

There are four Drawing Settings that affect the appearance of bonds: Line Width, Bold Width, Hash Spacing, and Bond Spacing. These settings apply simultaneously to all the bonds in the active document. Changes made to any of these settings affect the current document only. See "Saving Customized Settings" in *Chapter 1, ChemDraw Basics*.

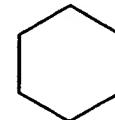
Drawing Settings Guide

Line Width

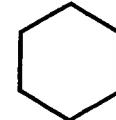
The thickness of all bonds, lines and arrowheads is specified in the box labeled "Line Width" in the Drawing Settings dialog box.



0.5 Point



1 Point



1.5 Point

To change the Line Width:

- From the File Menu, choose Drawing Settings.
- Type a value in the Line Width box, then click the OK button.

Bold Width

The thickness of bold, hashed and wedged bonds is specified in the box labeled "Bold Width" in the Drawing Settings dialog box.



2 point



4 Point



8 Point

To change the Bold Width:

- Enter a bold width in the Bold Width box, then click the OK button.

The Bold Width setting must be greater than the Line Width setting.

This change affects the current document only. See "Saving Customized Settings" in *Chapter 1, ChemDraw Basics* to learn how to make the change permanent.

Hash Spacing

The spacing between the hash marks in hashed bonds and the dash marks in dashed arrows in curves is specified in the box labeled "Hash Spacing" in the Drawing Settings dialog box.



2 Point



2.5 Point



3 Point

To change the Hash Spacing:

- Type a Hash Spacing in the Hash Spacing box, then click the OK button.

Bond Spacing

The spacing between bonds in double and triple bonds is measured as a percentage of the bond length. It is specified using the Bond Spacing control arrows in the Drawing Settings dialog box. You can set the bond spacing from 1 to 100% of the bond length.



10%



14%



18%

To change the bond spacing:

- Click the up or down Bond Spacing arrow to increase or decrease the bond spacing.

This change affects the current document only. See "Saving Customized Settings" in Chapter 1, *ChemDraw Basics* to learn how to make the change permanent.

EDITING BONDS

You can modify the appearance of chemical structures by changing bond types, moving atoms, and layering bonds.

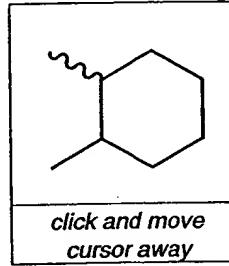
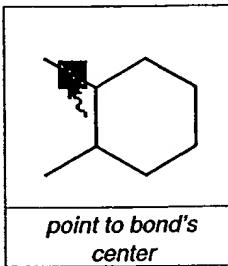
Changing Bond Types

To change a single bond from one type to another:

- Select a bond tool.
- Point at the center of an existing bond and click.

The bond that you click changes to the new bond type.

Figure 3-25 Changing a bond type



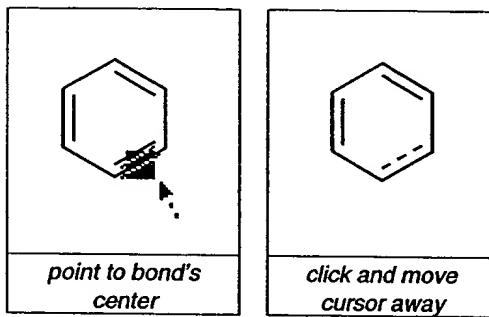
Double Bonds

To change one type of double bond to another:

- Select the Bold, Dashed or Solid Bond tool.
- Point to one of the bonds in the double bond.
- Click the bond.

The double bond changes to the new bond type. One of the bonds in the double bond is always a solid or dashed bond. Note, if you click a Tautomeric bond (solid/dashed) a second time with the dashed bond tool, you create an aromatic double bond (dashed/dashed).

Figure 3-26 Changing the bond type of a double bond



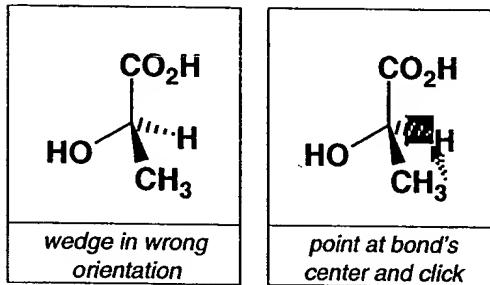
Orientation of Wedged and Dative Bonds

When you draw or change a bond to a wedged or dative bond, the orientation of the bond is chosen appropriately. However, if the orientation is the opposite of what you want:

- Click the dative or wedged bond with the tool used to create it.

The dative or wedged bond is changed to the opposite orientation.

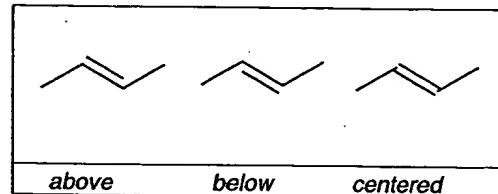
Example 3-27 Changing the orientation of a wedged bond



Alignment of Double Bonds

The bonds in a double bond can have any one of three alignments relative to other bonds: above, below or centered.

Figure 3-28 Alignment of lines in double bonds

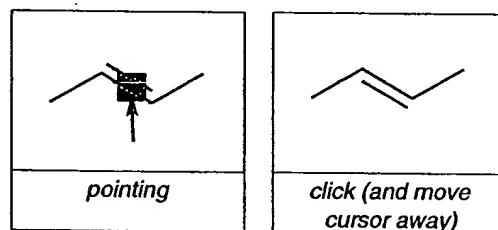


To change the alignment of a double bond:

- Select the bond tool used to create the existing double bond.
- Click the center of the double bond.
- Click one line of the double bond again to change to the next alignment.

The double bond shifts so that one of the lines of the bond moves to the other side of the structure.

Figure 3-29 Changing the alignment of a double bond



Moving Atoms

To move an atom in a chemical structure:

- Select a bond tool.

You can use any of the bond tools to move an atom within acyclic or cyclic structures (you cannot use a ring tool to perform this type of operation).

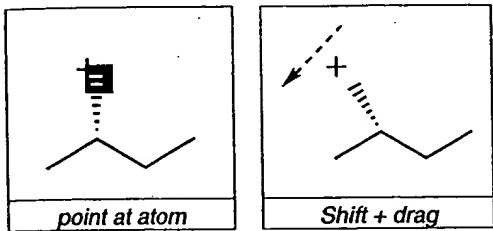
- Point at the atom to move.

A highlight box appears over the atom.

- Shift+drag the atom.

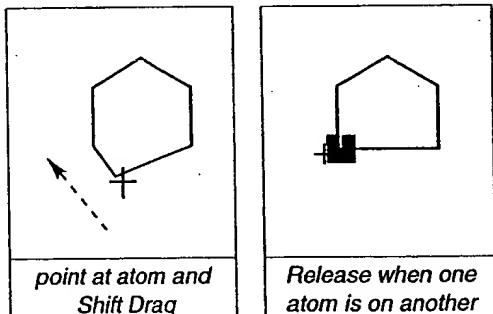
If you move an atom that has only one bond attached to it while Fixed Lengths is on, the atom will rotate around the other atom of the bond; the bond will not lengthen or shorten. If you move an atom that is part of two or more bonds, the atom will follow the pointer whether or not Fixed Lengths is on, and the bonds will stretch.

Figure 3-30 Moving an atom



If you drag one atom on top of an adjacent atom, the bond between the atoms disappears. This is useful for converting a 6-membered ring into a 5-membered ring.

Figure 3-31 Moving an atom onto another



NOTE: In addition to moving an atom with a bond tool, you can also move atom(s) using the Selection tool. For more information refer to "Moving Atoms" Chapter 7, Working with Selections.

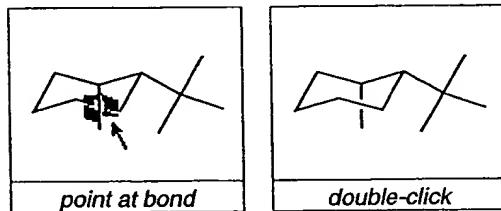
Bond Crossings

When one bond crosses another, white space is used to indicate which bond is in front of the other.

To change which bond is in front:

- Select any bond tool.
- Double-click the bond that you want to bring to the front.

Figure 3-32 Changing the front to back ordering of a bond



NOTE: You can also layer bonds using the Bring to Front and Send to Back commands. For a discussion of these commands, see Chapter 12, Working with Page Layout.

NOTE: You can magnify your view to make changing the bond layering easier. For more information, see "Perspectives" in Chapter 12, Working with Page Layout.

Drawing Settings Guide

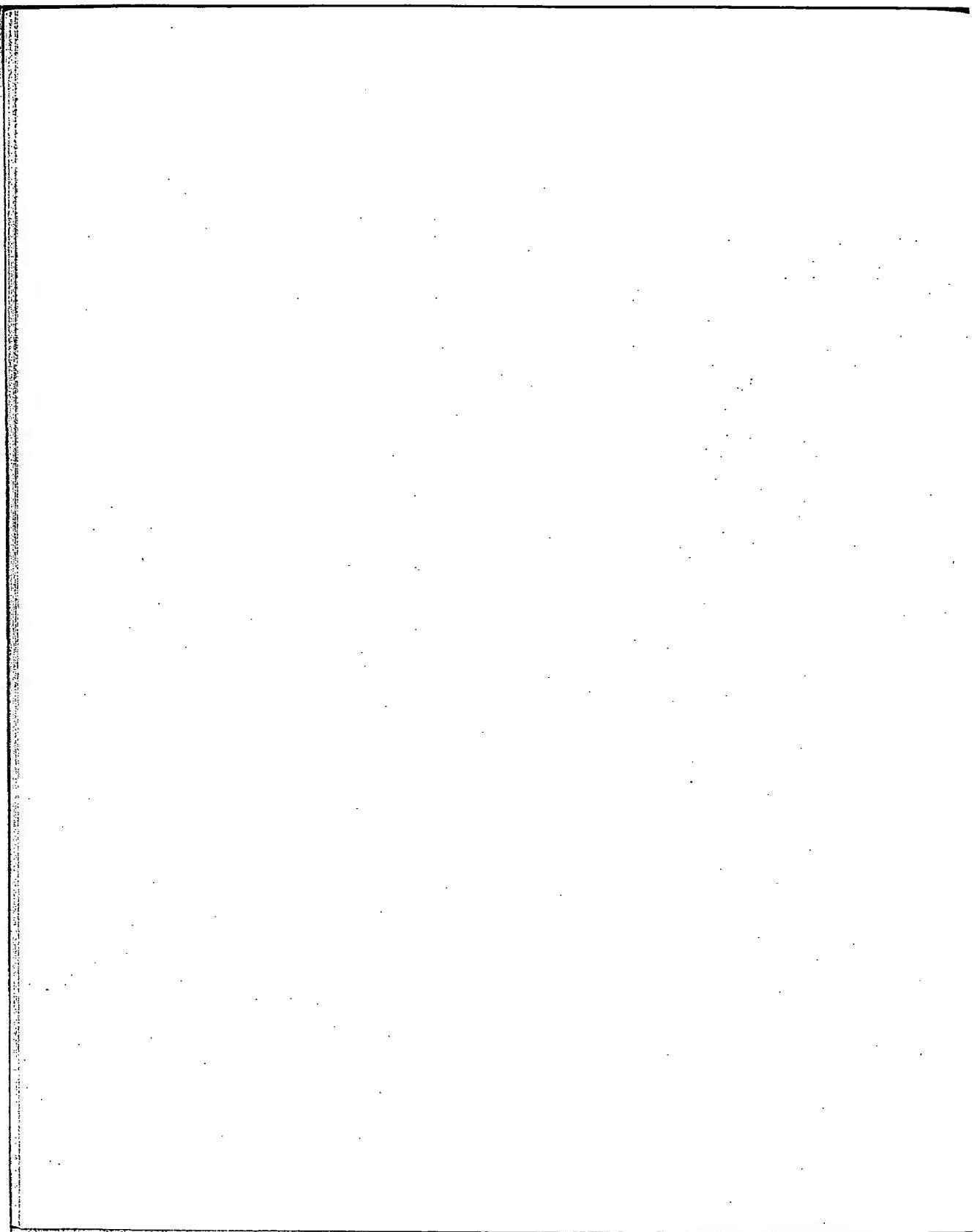
Margin Width

To adjust the white space that surrounds a bond in the region where one bond crosses another:

- Choose Drawing Settings from the File menu.
- Enter a value in the Margin Width box.
- Click the OK button.

The units used are those specified in the Preferences dialog box.

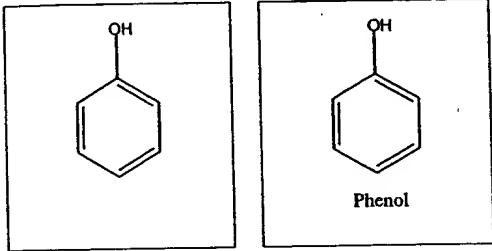
This change affects the current document only. See "Saving Customized Settings" in Chapter 1, ChemDraw Basics to learn how to make the change permanent.



Chapter 4, Captions and Atom Labels

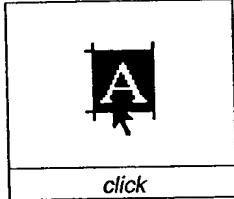
There are two kinds of text in *ChemDraw*: caption text and atom label text. Caption text is used to create annotations, chemical names, chemical formulas, page titles, and information in tables. Atom label text is used to identify atoms and substructures by their chemical symbols and formulas. Also see *Chapter 8, Advanced Drawing Techniques*, to learn how to use HotKeys to quickly label atoms, and how to check the chemistry of captions and atom labels.

Figure 4-1 Atom labels and captions



Both caption text and atom label text are created using the Text tool. The location of the created text, in empty space or on an atom, determines the type of text and the available justifications.

Figure 4-2 Text tool



To select the Text tool:

- Click the Text Tool icon in the Tools palette.

Text in a single caption or atom label can be edited using the Text tool. Other manipulations, especially those done simultaneously on several captions or atom labels, can be performed using the Selection tool. To learn more about the Selection tool, see *Chapter 7, Working with Selections*.

Two useful shortcuts when working with text are as follows:

To quickly switch from the Text tool to the Selection tool:

- Press **Ctrl+Alt+Tab (Windows)** or **Command+Tab (Macintosh)**.

The text box is automatically selected when you switch to the Selection tool.

To quickly switch from the Selection tool to the Text tool when a caption or atom label is selected:

- Press **Ctrl+Alt+Tab (Windows)** or **Command+Tab (Macintosh)**.

The Text tool is selected and the text box is opened for editing.

To select multiple atom labels or captions with the Selection tool:

- **Shift+click** the atom labels or captions.

Preferences Guide (Macintosh)

Use Bitmap Fonts When Available

When text appears in a document on the screen, it can appear using either a bitmap or a TrueType font. To use Bitmap fonts if they are available:

- From the File menu, choose Preferences.
- Select the **Use Bitmap Fonts When Available** checkbox.

Text drawn using Bitmap fonts looks better and appears more quickly than text drawn using TrueType fonts. However, the size and position of text drawn using Bitmap fonts will change somewhat when printed. For accurate correspondence between what you see on the screen and what is printed, deselect **Use Bitmap Fonts When Available**. This change affects all documents.

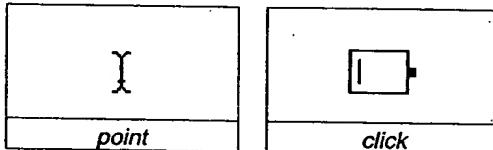
CAPTIONS

To create a caption:

- Select the Text tool.
- Point in an empty space in a document window.

A Caption text box with a flashing insertion point appears.

Figure 4-3 Creating a text box



- Type a caption.

The text box widens as you type to accommodate the caption.

- To create a new line, press the Enter (or Return) key.

You can also click outside the Caption text box in a document window to close the current Caption text box and open a new Caption text box.

NOTE: You can verify the chemical significance of captions using the Check Structure command. See Chapter 8, Advanced Drawing Techniques, for more information. In addition, you can use the Analyze Structure command to calculate information about the caption. See Chapter 8, Advanced Drawing Techniques, for more information. Captions must be formatted in "Formula" style for these commands to work for captions.

Preferences Guide

Require Ctrl+Enter (or Option+Return) to Create New Line

Within a Caption text box, the standard way of creating a new line is to press the Enter (or Return) key.

To close the text box you need to click anywhere outside the text box, press the Enter key (or Return key) or select another tool. If you prefer to use the Return key to close the Caption text box, and create a new line by pressing Ctrl+Enter (Windows) or Option+Return (Macintosh), do the following:

- From the File menu, choose Preferences.

Under the option "Require Ctrl+Enter (or Option+Return) to Create New Line".

- Select the **Captions** check box and click the OK button.

This change affects all documents.

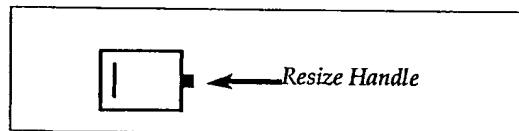
Caption Width

To change the width of a caption:

- Select a caption using the Text tool.

The Caption text box appears around the caption. On the right side of the text box is a **Resize handle**.

Figure 4-4 Text box resize handle



- Drag the Resize handle.

The point at which the text wraps is adjusted as you drag the Resize handle.

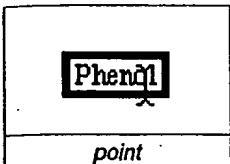
Editing the Contents of a Caption

To open a caption for editing:

- Select the Text tool.
- Point at a caption and click to open the text box.

The caption text is highlighted within the Caption text box.

Figure 4-5 Selecting captions for editing



To open a caption for editing by using the Selection tool:

- Select a single caption using the Selection tool.
- Press **Ctrl+Alt+Tab** (Windows) or **Command+Tab** (Macintosh).
- Or, select the Text tool.

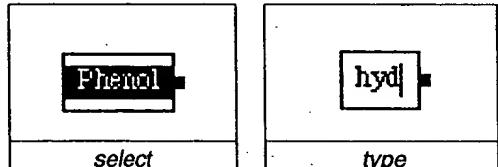
The Text tool is selected and the caption is opened. If more than one caption is selected, all captions are deselected.

To change all of the highlighted text within an open text box:

- Type the new caption text over the highlighted text.

The highlighted text disappears as you type the new caption.

Figure 4-6 Replacing selected text



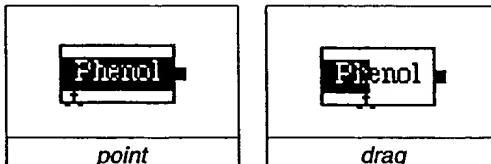
If not all the text is highlighted, and you want to select all of the caption text:

- From the Edit menu, choose **Select All**.

To change part of the caption text:

- Drag the insertion point over a part of the caption.

Figure 4-7 Replacing part of the text



NOTE: You can use the **Delete** key (or the **Forward Delete** key if available) to delete the character directly after the Insertion point. On the Macintosh, you can also delete a word directly after the Insertion point by pressing **Option+Forward Delete**.

Caption Fonts, Sizes and Styles

Each new caption that you create has the Font, Size and Style that is specified in the Text Settings dialog box. You can change these settings so that all new captions you type will use these new values, or you can change individual captions by using the commands in the Text menu.

To change the Font, Size or Style for an entire caption, or for several captions:

- Select the caption(s) using the Selection tool.

To change only a part of a single caption you must use the Text tool:

- Select part of the caption with the Text tool.

Caption Font

To specify a font for a selected caption:

- From the **Font** submenu within the Text menu, choose a Font.

Caption Size

To change the size for a selected caption text:

- From the **Size** submenu within the Text menu, choose a Size.

If the size you want is not listed in the Size submenu:

- From the Size submenu, choose Other.
- Type a number in the Other Size dialog box.
- Click the OK button.

Only one alternate size is listed in the Size menu. This alternate size changes depending on the selection.

NOTE: If the captions you select have more than a single font or size, a hyphen appears next to each font or size that is contained within the selection. Choosing a new font or size in this instance will change all of the selected text to the new font or size.

Style

The Style submenu contains three items in addition to those found normally in the Macintosh Style menu: Superscript, Subscript, and Formula. The Superscript style reduces the font size of caption text by twenty-five percent and raises its baseline. The Subscript style reduces the caption text by twenty-five percent and lowers the baseline. When you apply the Formula style, numbers are subscripted automatically, for instance, C₆H₆.

To specify the style of caption text:

- From the Style submenu within the Text menu, choose a style.

You can apply several styles to the same selected caption(s), for instance, Formula, Bold and Italic. You can also apply multiple styles to different portions of a single caption.

NOTE: If the captions you select have more than one style, a hyphen appears next to each style that is not applied to the entire selection. A checkmark appears next to each style that applies to all of the selected text. Making a choice (except for Plain) in this instance will add the new style choice to all of the selected captions. Previously applied styles are not affected.

Text Settings Guide

New Caption Font, Size and Style

To change the font, size and styles for new captions:

- From the File menu, choose Text Settings.
- Choose a Font, Size and Style in the section labeled "New Captions".

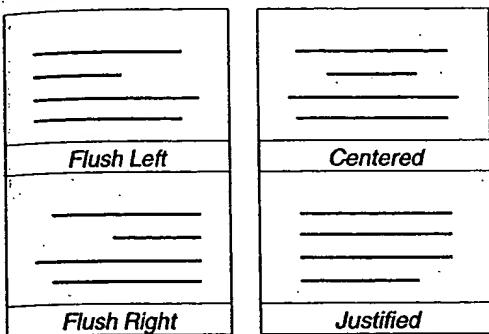
These settings take effect for all new captions that you type in the current document window. To use these settings in new documents you can save them in a stationery pad. See "Saving Customized Settings" in Chapter 1, ChemDraw Basics.

This change affects the current document only. See "Saving Customized Settings" in Chapter 1, ChemDraw Basics to learn how to make the change permanent.

Caption Justification and Line Spacing

All new captions you create are Flush Left and the line spacing is chosen automatically unless you specify otherwise by using the Justification and Line Spacing commands in the Text menu. All text in a single caption must have the same Justification and Line Spacing. There are four justifications available in the Text menu: Flush Left, Centered, Flush Right, and Justified. Flush Left creates left-justified caption text; Centered creates centered caption text; Flush Right creates right-justified caption text; and Justified creates right-left justified caption text.

Figure 4-8 Text justification



To specify the justification of caption(s):

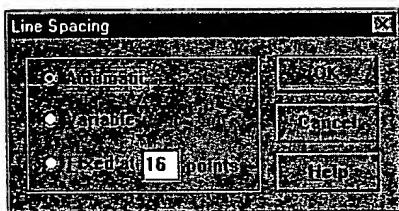
- Select a caption(s) using the Selection tool.
- From the Text menu, choose a justification.

To specify the spacing between different lines of a caption:

- Select a caption(s) using the Selection tool.
- From the Text menu, choose Line Spacing.

The Line Spacing dialog box appears.

Figure 4-9 Line Spacing dialog box



There are three ways to specify the Line Spacing: Automatic, Variable, and Fixed. Caption text with automatic line spacing has consistently spaced lines of text; the spacing is based on the size of the largest character in the caption. Captions with variable line spacing have lines of text with different spacing. In this case, the spacing is based on the largest character in each line. Captions with fixed line spacing have consistently spaced lines that you specify. Unless you specify otherwise, caption text has automatic line spacing.

To specify Automatic or Variable line spacing:

- Select the Automatic or Variable button.

To specify a Fixed line spacing:

- Select the Fixed button.
- Type a value in the text box labeled "Fixed at".

NOTE: The line spacing of ChemDraw version 2.x documents opened within ChemDraw version 4.0 is automatically set to Fixed Line spacing to maintain vertical alignment.

ATOM LABELS

To place an atom label on an atom:

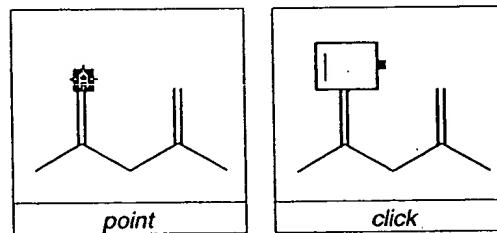
- Select the Text tool.
- Point to an atom.

The pointer changes when it is positioned correctly over an atom to indicate that you will create an atom label rather than a caption.

- Click the atom.

An Atom Label text box appears over the atom.

Figure 4-10 Creating an atom label



- Type an atom label.

Numbers are automatically subscripted. Letters in an atom label are positioned on a bond depending on the justification you have chosen (see "Atom Label Justification" later in this chapter). Numbers, leading open parentheses and trailing closed parentheses are ignored in the positioning of atom labels.

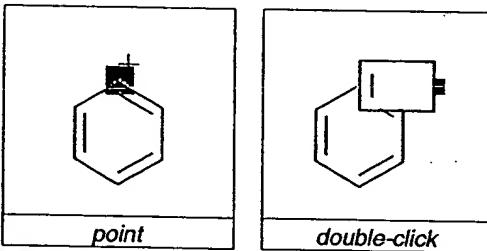
- Press Enter (or Return) to close the Atom Label text box.

You can also click outside the current Atom Label text box on another unlabeled atom to open a new Atom Label text box.

To label an atom using a bond or ring tool

- Point to an atom and double-click.

Figure 4-11 Creating an atom label using a bond tool



NOTE: As an alternative to creating atom labels using the Text tool, you can use HotKeys to label atoms. In addition, you can label atoms using Nicknames which are text representations of substructures. You can also verify the chemical significance of atom labels using the Check structure command. See "Nicknames" in Chapter 8, Advanced Drawing Techniques, for more information.

Preferences Guide

Require Ctrl+Enter (Windows) or Option+Return (Macintosh) to Create New Line

In an Atom Label text box, the standard way of creating a new line is to hold down the Ctrl key (Windows) or Option key (Macintosh) and press the Enter (or Return) key. To close the text box, press the Enter (or Return) key. If you prefer to use the Enter (or Return) key to add a new line and to close the Atom Label text box by clicking outside the text box.

You can change this preference as follows:

- From the File menu, choose Preferences.
- Deselect the Atom Labels check box (under this option).
- Click the OK button.

This change affects all documents.

Isotopes

ChemDraw will automatically recognize isotopes¹ if they are properly labeled with superscripts, e.g., ¹³C, ¹⁵N, and ⁸¹Br.

To label an atom with an isotope:

- Open a text box on an atom position using the Text tool or by double-clicking with a Bond tool.
- Type an isotope, e.g. "13C".
- Using the Text tool, select the isotopic mass, "13".
- From the Text menu, in the Style submenu, select Superscript.

Copying and pasting will transfer this isotope information to the Clipboard.

NOTE: ChemDraw contains extensive information (reproduced by permission of CRC Press, Inc.) about known isotopes. It is extremely unlikely that you would ever need to change this information, but if you do, you may edit the Isotopes table (Macintosh) or Isotopes.txt (Windows) with your favorite text editor.

¹ Adapted from the *Table of Isotopes* data, in the CRC Handbook of Chemistry and Physics, 77th Ed., Lide, D.R., Editor-in-Chief, CRC Press, Boca Raton, Florida, ©1996. With permission.

Figure 4-12 Creating an isotope label

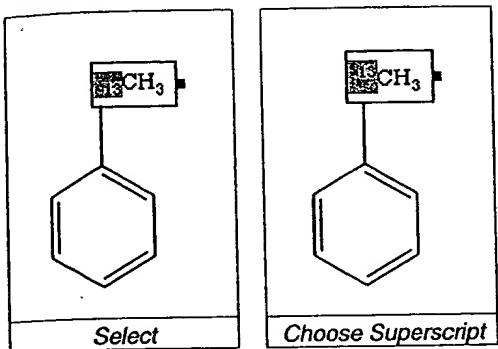
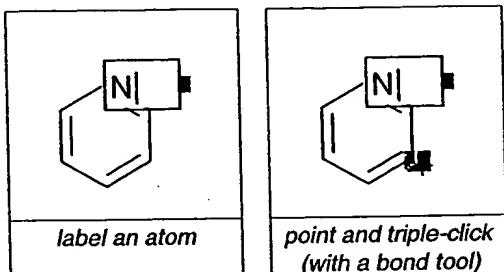


Figure 4-13 Repeating an atom label



Charges

To label an atom with an associated charge:

- Open a text box on an atom position using the **Text tool** or by double-clicking with a **Bond tool**.
- Type a plus or minus sign after the atom you want to label with a charge.
- (Optional) From the **Style** submenu in the **Text menu**, choose **Superscript**.

Repeating an Atom Label

To label several atoms with the same atom label:

- Select the **Text tool**.
- Label a single atom.
- Double-click an atom to repeat the previous label.

Alternatively, you can label an atom while using a bond or ring tool:

- Select a **bond tool**.
- Double-click an atom.

To repeat the label:

- Triple-click an atom to repeat the previous label.

This method can be used with any of the bond tools, ring tools and the Acyclic Chain tool.

Atom labels are always in the frontmost object layer in the document window and are therefore always layered on top of bonds. See "Layering Objects" in *Chapter 12, Working with Page Layout*, for more information.

Drawing Settings Guide

Margin Width

The white space surrounding the atom label can be adjusted so that more or less of the attached bond is hidden.

To adjust the white space:

- From the **File menu**, choose **Drawing Settings**.
- Type a new value in the **Margin Width** box.
- Click the **OK** button.

Editing Atom Labels

To edit an atom label:

- Click an existing label using the **Text tool** or double-click using a **bond** or **ring tool**.

The highlighted atom label text appears within the Atom Label text box.

If the text is not all highlighted, and you want to select all of the atom label:

- From the **Edit menu**, choose **Select All**.

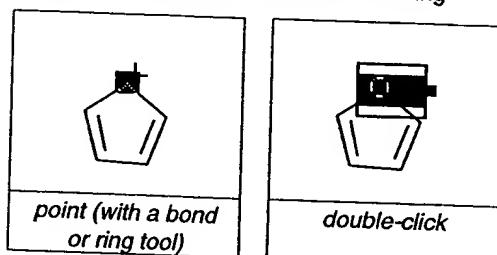
To edit part of the atom label:

- Drag the insertion point over part of the atom label.
- Type the new characters.
- Press Enter (or Return) to close the Atom Label text box.

You can also open an atom label for editing as follows:

- Double-click an existing atom label using a bond, ring, or chain tool.

Figure 4-14 Opening a text box for editing



Deleting an Atom Label

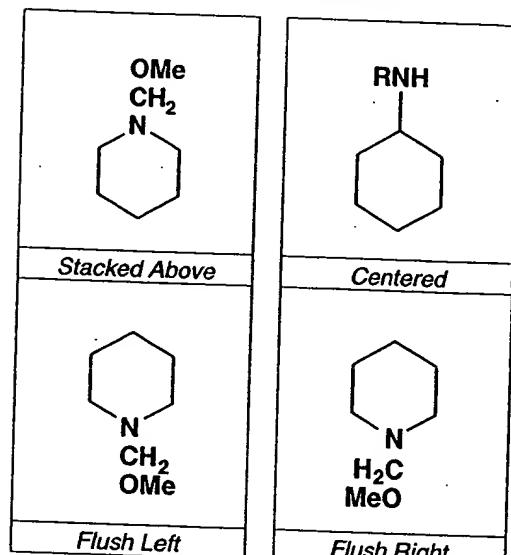
To delete an atom label, leaving the underlying bond(s) unchanged:

- Click the atom label using the Eraser tool or use the "space" HotKey.

Atom Label Justification

With *ChemDraw*, you can use the Automatic, Centered, Flush Left, Flush Right, and Stacked Above justifications from the Text menu to create labels that identify atoms and functional groups in your chemical structure without obscuring any bonds or other atom labels. Below are examples of the atom label justifications available ("Justified" is not available for atom labels).

Figure 4-15a Atom Label justification

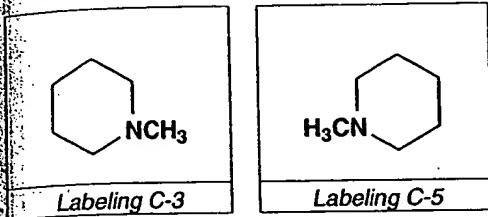


Automatic Justification

Atom labels can be justified automatically. To correctly position the atom label, the label is broken up into tokens. A token consists of an uppercase letter followed by any numbers or lowercase letters. The first token is attached to the atom and the rest of the label is positioned so that it does not obscure other parts of the chemical structure.

To create N-methylpiperidine, label an atom in cyclohexane with the atom label "NCH₃", which contains the three tokens, "N" and "C" and "H₃". If you label C3, the tokens are placed from left to right since there are bonds to the left of the atom. If you label C5, the tokens are placed from right to left since there are bonds to the right of the atom:

Figure 4-15b Creating N-methylpiperidine

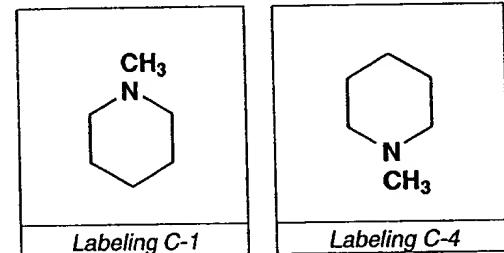


In ChemDraw Pro, you can force an entire multi-atom label to be a token by defining it as a Nickname. This prevents the label from flipping when applied to the left side of a structure.

For instance, If you define the Nickname "CH₃", and label C-5 with the combined label and nickname "NCH₃", the final orientation will be "CH₃N" rather than "H₃CN". In this case, the Nickname, "CH₃", is a token (also see "Nicknames" in Chapter 8, Advanced Drawing Techniques).

If you label C-1, the second and third tokens are placed above the first token since there are bonds below the atom. If you label C-4, the second and third tokens are placed below the first token.

Figure 4-15c Creating N-methylpiperidine



Preferences Guide

Automatic Atom Labels

To set the default atom label justification to Automatic:

- From the File menu, choose Preferences.
- Select the Automatic Atom Labels check box, then click the OK button.

Each time a new atom label is created, it will be automatically justified.

This change affects all documents.

Stacked Above

To create an atom label using the Stacked Above justification.

- Select an atom to label.
- From the Text menu, choose Stacked Above.
- Type the top row of characters.

To create a new line:

- Press Ctrl+Enter (or Option+Return) to create a new line.
- Type the second line of characters.

The atom label appears as a stack.

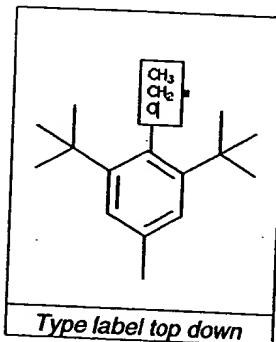
- Repeat this procedure until the entire stacked atom label is created.

To close the Atom Label text box:

- Press Enter (or Return).

The bonds are drawn to the left-most character in the last row that you typed.

Figure 4-16 Stacked Above labels



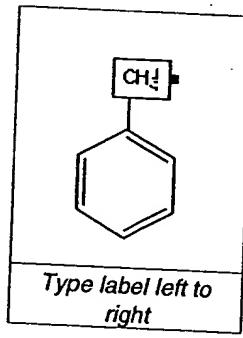
Type label top down

Flush Left Justification

To create an atom label using the Flush Left justification:

- Select an atom to label.
- From the Text menu, choose Flush Left.
- Type the first row of characters.
- Press Ctrl+Enter (or Option+Return) to create a new line.
- Repeat this procedure until you have typed all rows in the atom label.
- Press Enter (or Return) to close the Atom Label text box.

Figure 4-17 Flush Left labels



Type label left to right

Preferences Guide

Automatic Atom Labels

To set the default atom label justification to be other than automatic:

- From the File menu, choose Preferences.
- Deselect the Automatic Atom Labels check box.
- Click the OK button.

Each time a new atom label is created, it will be justified to the left, right, or stacked above, depending on the position of the bonds to that atom.

This change affects all documents.

Flush Right Justification

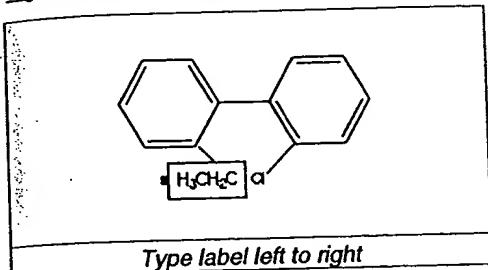
To create an atom label using the Flush Right justification:

- Select an atom to label.
- From the Text menu, choose Flush Right.
- Type the first row of characters.

When an atom label is justified Flush Right, the last uppercase character in the first line you type will be attached to the bond.

- Press Ctrl+Enter (or Option+Return) to create a new line.
- Repeat this procedure until you have typed all the rows in the atom label.
- Press Enter (or Return) to close the Atom Label text box.

Figure 4-18 Flush Right labels



Centered Justification

To create an atom label that has Centered justification.

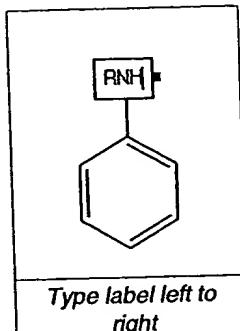
- Select an atom to label.
- From the Text menu, choose Centered.
- Type a row of characters so the center character is the character you want connected to the bond.

Centered justification requires that the same number of characters (including numbers) is on each side of the atom label joining the bond. For instance, CH₃NCH₃, will be centered on the nitrogen, whereas RNCH₃ will be centered on the carbon.

- Press Ctrl+Enter (or Option+Return) to create a new line, if necessary.
- Type the second line of characters.

NOTE: for precise control of atom label alignment, see "Multi-attached Labels" in Chapter 8, Advanced Drawing Techniques.

Figure 4-19 Centered labels



Atom Label Line Spacing

You can adjust the spacing between the lines of an atom label using the Line Spacing command in the Text menu in the same manner as for captions. Variable line spacing is the default for atom labels. Refer to "Caption Label Justification and Line Spacing" earlier in this chapter for a detailed discussion of the Line Spacing command and the associated options available in the Line Spacing dialog box.

NOTE: The line spacing of ChemDraw version 2.x documents opened within ChemDraw version 4.0 is automatically set to Fixed Line spacing to maintain vertical alignment.

ENTERING NON-ROMAN TEXT

ChemDraw uses standard methods for entering all types of text, including the Greek characters and other symbols that are common to chemistry. To enter Greek characters:

- Click in a text box with the text tool
- From the Font submenu in the Text menu, choose Symbol (Windows users may need to choose the Other menu item within this submenu, and select the Symbol font from there)
- Enter your text. For example, an "a" is a lower-case alpha, a "P" is a capital pi.

- If you want to enter additional non-Greek text in the same text box, go back to the Font submenu and re-select the font that was selected previously.

To enter a degree symbol:

- Click in a text box with the text tool

Macintosh

- Press option+shift+8

Windows

- Make sure the Num Lock key is pressed on your keypad
- Hold down the ALT key
- On the keypad, type the four numbers 0,1,7,6 in succession
- Release the ALT key

NOTE: The characters available differ in different fonts. A list of all characters available in each font – and what to type to get them – is available in the KeyCaps menu item of the Apple menu (Macintosh) or the Character Map application in your Accessories program group (Windows).

TEXT FORMAT

ChemDraw uses default format settings that determine the font, size and style of captions and atom labels that you type. You can change the formatting by choosing new formats before you type, or by selecting text and applying the new formats after you type. The format can be changed in two ways:

1. Using the Font, Size, and Style submenus.
2. Using the Format dialog box (Windows only).

NOTE: In addition, the Style can be changed using the key combinations listed to the right of the style command in the Style submenu, and the Size of selected text can be changed using the Resize handle or Scale dialog box using the Selection tool.

Alternatively, you can change the defaults for a particular document using the atom label or caption text settings commands. Changing atom label defaults affects all existing atom labels, as well as newly created atom labels within the active document. Changing caption defaults changes the format for all newly created captions in the active window.

Using the Font, Size and Style Submenus

The Font, Size and Style submenus located in the Text menu provides a quick way to change individual format options for captions and atom labels.

The Font submenu contains fonts installed in your system, and lists the most recently used fonts. An "Other" command provides a way to add a font that is not currently listed.

The Size submenu contains the font sizes available, and lists the most recently used sizes. An "Other" command provides a way to add a size that is not currently listed.

The Style submenu contains three additional baseline styles not normally found in Style menus: Superscript, Subscript, and Formula. The Superscript style reduces the font size of caption text by twenty-five percent and raises its baseline. The Subscript style reduces the caption text by twenty-five percent and lowers the baseline. When you apply the Formula style, numbers are subscript automatically, for instance, C₆H₆. The default for atom labels normally contains the Formula style.

To change the Font, Size or Style using a submenu:

- Before you begin typing, choose the font style and size that you want from the submenus.
- Or, select the caption(s) using the Selection tool, or individual captions or atom labels with the Text tool.
- From the Size and Font submenus, choose the font style and size.

NOTE: If the captions you select have more than a single font or size, a partial selection mark appears next to each font, size or style that is contained within the selection. Choosing a new font or size in this instance will change all of the selected text to the new font or size. Choosing a style will add the new style to all of the selected captions or atom labels without affecting styles previously applied.

If the Font you want is not currently displayed in the submenu:

- From the Fonts submenu, choose Other.

The Font dialog box appears.

- From the Font drop-down list box, choose a font.
- Type a number in the Other Size dialog box.
- Click the OK button.

If the Size you want is not currently displayed in the submenu:

- From the Size submenu, choose Other.

The Size dialog box appears.

- Type a number in the Other Size dialog box and click the OK button.

Using the Format Dialog Box (Windows Only)

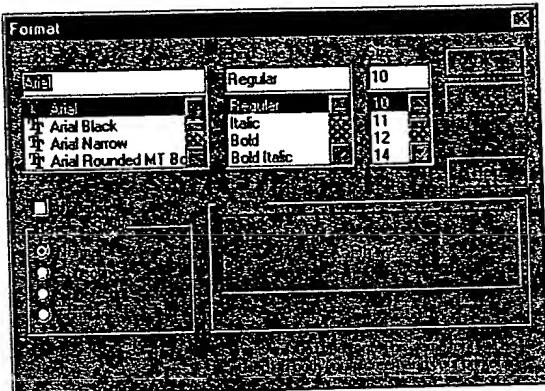
The Format command in the Text menu displays a dialog box where you can make several format changes at one time, rather than choosing individual formats from submenus.

To change the font, size and style using the format dialog box:

- Before you begin typing, choose Format from the Text menu.
- Or, select the multiple captions or atom labels using the Selection tool, or individual captions or atom labels with the Text tool.
- From the Text menu, choose Format.

The Format dialog box appears (Figure 4-20).

Figure 4-20 Format dialog box (Windows only)



- Select the Font, Size and Style options that you want to apply.
- Click the OK button.

The new formats are applied to the selection or to the new text you type.

Changing Default Settings

The default settings for caption and atom labels are changed using the Caption Text Settings and Label Text Settings commands in the File menu. The default settings are stored in the active document only. To use these settings in other documents you can save them in a Style Sheet. See "Saving Customized Settings" in Chapter 1, ChemDraw Basics.

Text Settings Guide

New Caption Font, Size and Style

To change the default font, size and styles for new captions:

- From the File menu, choose **Caption Text Settings**.

The Caption Text Settings dialog box appears.

- Select a **Font, Size and Style**.

These settings take effect for all new captions that you type in the active document window.

Atom Label Fonts, Size and Styles

To change the font, size and styles for all atom labels in the active document window (as well as any atom labels you create later):

- From the File menu, choose **Atom Label Text Settings**.

The Atom Label Text Settings dialog box appears.

- Select a **Font, Size and Style**.

Changing the size of atom labels in the Text Settings dialog box changes the size of each atom label in the active document window by the following scale factor:

$$\text{new atom label size} = \left(\frac{\text{new default size}}{\text{old default size}} \right) \text{old atom label size}$$

TABLES

With *ChemDraw* you can create tables of text using the Tab key in conjunction with the Text tool.

Creating the First Row (column headings)

To create the first row and establish the columns of a table:

- Select the **Text tool**.
- Click in a document window where you want the table to start.

- Choose a style, font and size from the appropriate submenu in the **Text** menu and then type a caption.

- Press **Tab**.

A second caption text box appears.

- Choose a style, font and size from the appropriate submenu in the **Text** menu and then type a second caption.

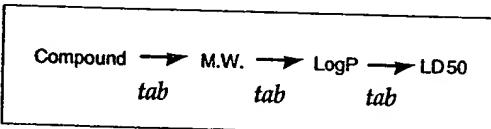
The second column is placed 20 points (20/72 inch, 0.71 cm) to the right of the first.

- Press **Tab** again to create a third column, and so on.

NOTE: The style, font and size that you set in each column will be maintained in all the rows that follow. For example, if column one is bold and column two is italic, the next row will automatically have column one as bold and column two as italic.

The following diagram illustrates the creation of new columns using the Tab key.

Figure 4-21 First row



To change the spacing between columns while editing a caption:

- Press **Ctrl+Alt+Tab** (Windows) or **Command+Tab** (Macintosh) or select the **Selection tool**.

The caption is automatically selected with the Selection tool.

- Press **Right** (or **Left**) **Arrow**.

This moves the selected caption to the right (or left) 1 point at a time.

To move 10 points at a time:

- Press **Ctrl+Right** (or **Left**) **Arrow** (or **Option+Left Arrow**).

To return to the Caption text box after completing the spacing change:

- Press **Ctrl+Alt+Tab** (Windows) or **Command+Tab** (Macintosh) or select the **Text tool**.

To create another column with this same spacing as the previous:

- Press **Tab**.

A third caption text box appears, and so on.

Creating a New Row

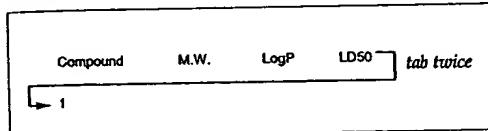
To start a new row that is exactly aligned with the first:

- Press **Tab** twice at the end of a row.

A caption text box appears exactly aligned under the first caption positioned exactly 20 points below the first caption in the first row.

The following diagram illustrates the creation of a new row.

Figure 4-22 Creating a new row



To change the spacing between rows as you create the table:

- Press **Ctrl+Alt+Tab** (Windows) or **Command+Tab** (Macintosh) when you are editing the first caption in a row, or, select the **Selection tool**.

The caption is automatically selected with the Selection tool.

- Press the **Down** (or **Up**) Arrow.

This moves the selected caption downwards (or upwards) 1 point at a time.

To move 10 points at a time:

- Press **Ctrl+Down** (or **Up**) Arrow (or **Option+Arrow key**).

To return to the Caption text box after completing the spacing change:

- Press **Ctrl+Alt+Tab** (Windows) or **Command+Tab** (Macintosh) or select the **Text tool**.

To continue and fill in the row with captions:

- Press **Tab** to create another caption in the row, then press **Tab** twice to begin a new row.

The spacing between the newest row and the row directly before it will have the same spacing that you specified between the previous two rows.

Adjusting Column Spacing

You can also use the Selection tool to adjust the column spacing as follows:

- Select all of the captions in a column using the **Selection tool**.

To change the spacing relative to the previous caption:

- Alt+drag (Windows) or Command+drag (Macintosh) the caption(s).

Holding down the Alt key (Windows) or Command key (Macintosh) constrains the movement to the X axis so that you can maintain the row alignment.

Adjusting Row Spacing

You can also use the Selection tool to adjust the row spacing as follows:

- Select the **Selection tool** and select all caption in a row.

To change the spacing between the selected row and the previous row:

- Alt+drag (Windows) or Command+drag (Macintosh) the captions down.

Holding down the Alt key (Windows) or Command key (Macintosh) constrains the movement to the Y axis so you can maintain the column alignment.

Moving Around Within Tables

To move around within an existing table.

- Select the Text tool and select a caption.

To move to the caption on the right and open it for editing:

- Press Tab, or, press Alt+Right Arrow (Windows) or Command+Right Arrow (Macintosh).

To move to the caption on the left and open it for editing:

- Press Shift+Tab, or, press Alt+Left Arrow (Windows) or Command+Left Arrow (Macintosh).

To move to the caption below and open it for editing:

- Press Alt+Down Arrow (Windows) or Command+Down Arrow (Macintosh).

To move to the caption above and open it for editing:

- Press Shift+Alt+Enter (or Shift+Command+Return), or, Press Alt+Up Arrow (Windows) or Command+Up Arrow (Macintosh).

Inserting a New Row

To insert a row:

- Select the Selection tool and select a row of captions.
- Alt+drag (Windows) or Command+drag (Macintosh) the selected row.

The Alt key (Windows) or Command key (Macintosh) constrains the movement to the Y axis to maintain the column alignment.

- Select the first caption in the row above or below the space you created.
- Ctrl+Alt+drag (Windows) or Option+Command+drag (Macintosh) to create a copy of the caption and position it in the empty space you created.

The placement of this copied caption sets the position of the inserted row.

To fill in the inserted row with caption text:

- Select the Text tool and select the first caption in the inserted row, and type new text.
- Press Tab to move to the second caption in the inserted row, and so on.

Chapter 5, Drawing Orbitals and Chemical Symbols

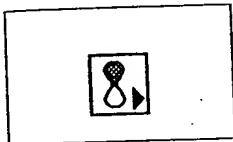
This chapter discusses two tools, the Orbital tool and the Chemical Symbols tool, that you can use to add to your structures. Both tools contain a palette of objects from which you can choose.

THE ORBITAL TOOL

The orbital tool is used to add orbitals to your chemical structures.

Orbitals are drawn so that its node appears first. To illustrate where the node for each orbital is, the remainder of this section illustrates each of the tools.

Figure 5-1 Orbital tool



Each orbital type is available in several fill patterns: white, gray, and black. Gray orbitals appear with grayscale shading on color and grayscale monitors and print with grayscale shading from PostScript printers when the Color/Grayscale option is selected in the Print dialog box.

Each orbital type is discussed separately below. While you draw an orbital, its length and angle relative to the X axis appears in the Message area.

You can constrain the length of an orbital by turning Fixed Lengths on in the Object menu. You can also constrain the angle of all orbitals to 15 degree increments relative to the X axis by turning on Fixed Angles.

NOTE: Orbitals are not part of the structure they are drawn near, and are therefore not selected if you double-click a bond, atom or atom label with the Selection tool. To group the orbitals with the structure, use the Group command in the Object menu. To learn more about grouping, see "Grouping" in Chapter 7, Working with Selections.

s-orbitals

To draw an s-orbital:

- Point to an atom where the orbital will be centered.
- Drag outward.

Figure 5-2 s-Orbitals

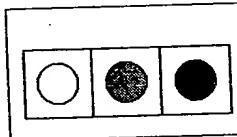
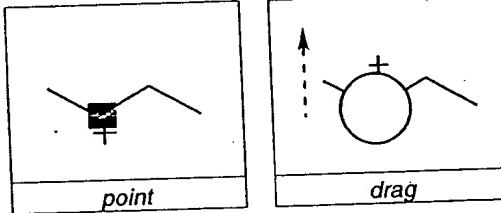


Figure 5-3 Adding an s-orbital

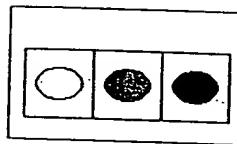


σ -orbitals

To draw a σ orbital:

- Point to an atom where the orbital will be centered.
- Drag outward along the long axis of the orbital.

Figure 5-4 σ -Orbitals



Single Lobe Orbitals

Single lobe orbitals are commonly used for indicating a lone pair. To draw a single lobe orbital:

- Point to an atom where the narrow end of the orbital is to be attached.
- Drag from the narrow end of the lobe to its wide end.

Figure 5-5 Single lobe orbitals

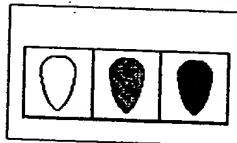
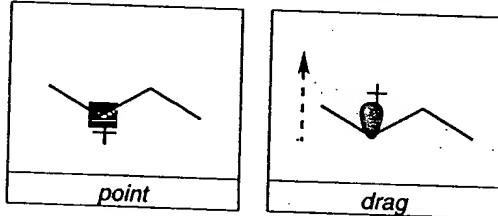


Figure 5-6 Adding a single lobe orbital



p-orbitals

To draw a p-orbital:

- Point to an atom where the node of the orbital is to be attached.
- Drag from the orbital node to the wide end of the filled lobe.

Figure 5-7 p-Orbital icons

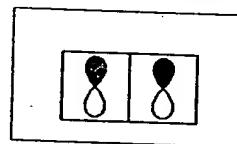
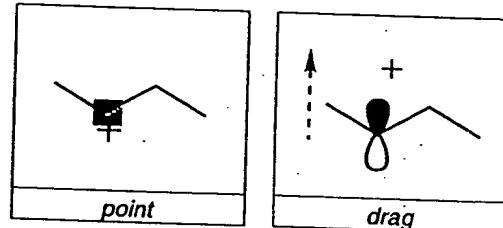


Figure 5-8 Drawing a p-orbital

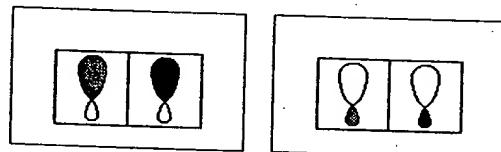


Hybrid-orbitals

To draw a hybrid orbital:

- Point to an atom where the node of the orbital is to be attached.
- Drag from the orbital node to the wide end of the major lobe of the orbital.

Figure 5-9 Hybrid orbitals

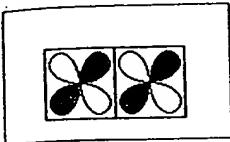


d-orbitals

To draw a d-orbital:

- Point to an atom where the node of the orbital is to be attached.
- Drag from the center of the orbital to the wide end of a filled lobe.

Figure 5-10 d-Orbitals

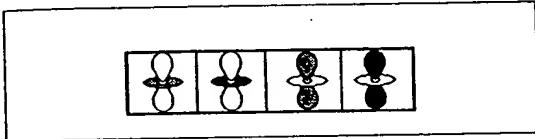


d_{z²}-orbitals

To draw a d_{z²}-orbital:

- Point to an atom where the node of the orbital will be attached.
- Drag from the center of the orbital to the wide end of a lobe.

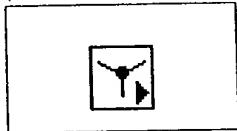
Figure 5-11 d_{z²}-Orbitals



THE CHEMICAL SYMBOL TOOL

The Chemical Symbol tool is used to add chemical symbols to your structure.

Figure 5-12 Chemical Symbol tool

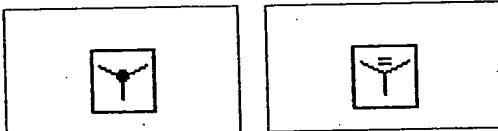


All chemical symbols are automatically grouped with the structure (or caption in formula style) to which it is closest. In addition, the symbols are included in any Analyze Structure or Check Structure function that you perform. See *Chapter 7, Working with Selections*, for more information about the Analyze and Check Structure command.

H-dot and H-dash

To represent a hydrogen that is coming out of the plane toward you along the Z axis, use the H-dot symbol. To represent a hydrogen that is directed backwards into the plane away from you along the Z axis, use the H-dash.

Figure 5-13 H-dot and H-dash

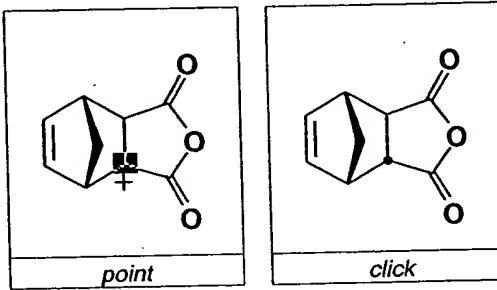


To draw an H-dot or an H-dash:

- Click an atom.

H-dots and H-dashes can only be drawn by clicking atoms.

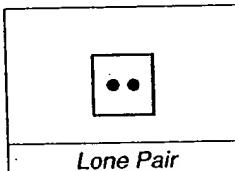
Figure 5-14 Adding an H-dot



Lone Pair

The lone pair symbol is used for indicating a lone pair of electrons common in Lewis structure representations.

Figure 5-15 Lone pair symbol



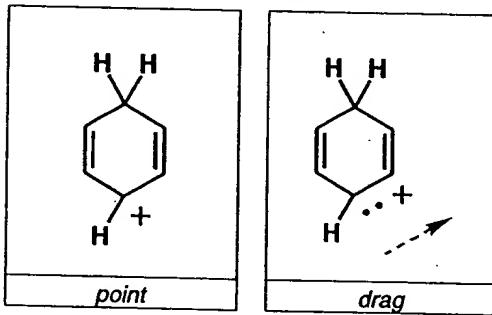
To draw a lone pair:

- Point to where you want one end of the lone pair to be positioned.
- Drag in the direction you want the end to be located and release the mouse button.

To quickly deposit a lone pair symbol in a horizontal orientation:

- Click in a document window.

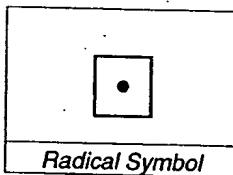
Figure 5-16 Adding a lone pair



Radical

The radical symbol is used for indicating a single non-bonded electron.

Figure 5-17 Radical symbol



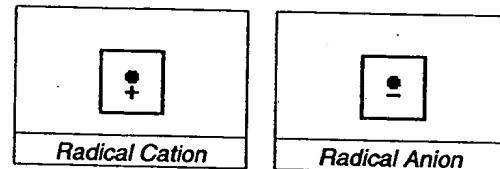
To draw a radical:

- Position the pointer next to an atom where you want the radical symbol to appear.
- Click to draw the symbol.

Radical Cation and Radical Anion

The charge radical symbols are used for representing radicals that are charged.

Figure 5-18 Radical cation and radical anion symbols



To draw a radical cation or radical anion symbol:

- Position the pointer next to an atom where you want the symbol to appear.
- Drag from the charge portion of the symbol to the radical portion of the symbol.

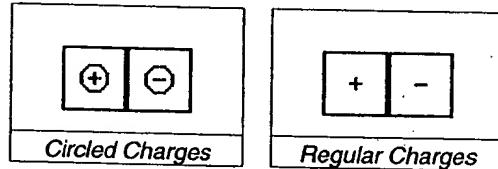
To quickly deposit a radical cation or radical anion symbol in a vertical orientation:

- Click to deposit the symbol.

Charges

The charge symbols are used for representing structures that are charged.

Figure 5-19 Negative and positive charge symbols

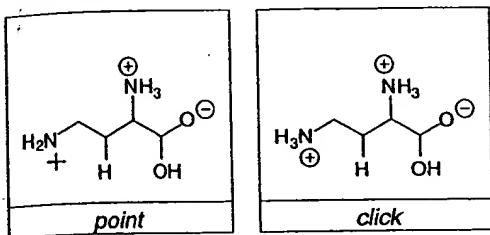


To draw a charge and associate it with a structure:

- Click next to the atom to which you want the charge to correspond.

Notice that the number of hydrogens increases or decreases as appropriate for the addition of the charge symbol.

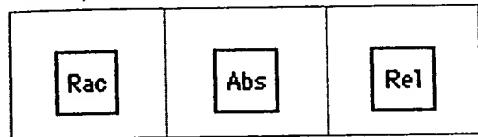
Figure 5-20 Adding a positive charge symbol



Stereochemical Flags

To remove ambiguity for structures where there is more than one possible stereochemical interpretation, you can assign a special flag symbol to the structure.

Figure 5-22 The Racemic, Absolute and Relative symbols



To draw a flag:

- Position the pointer next to the structure to which you want to assign the flag.
- Click to deposit the symbol.

The font and size for stereochemical flags matches the default Atom Label size for the document.

Editing a Symbol

To rotate a Chemical Symbol:

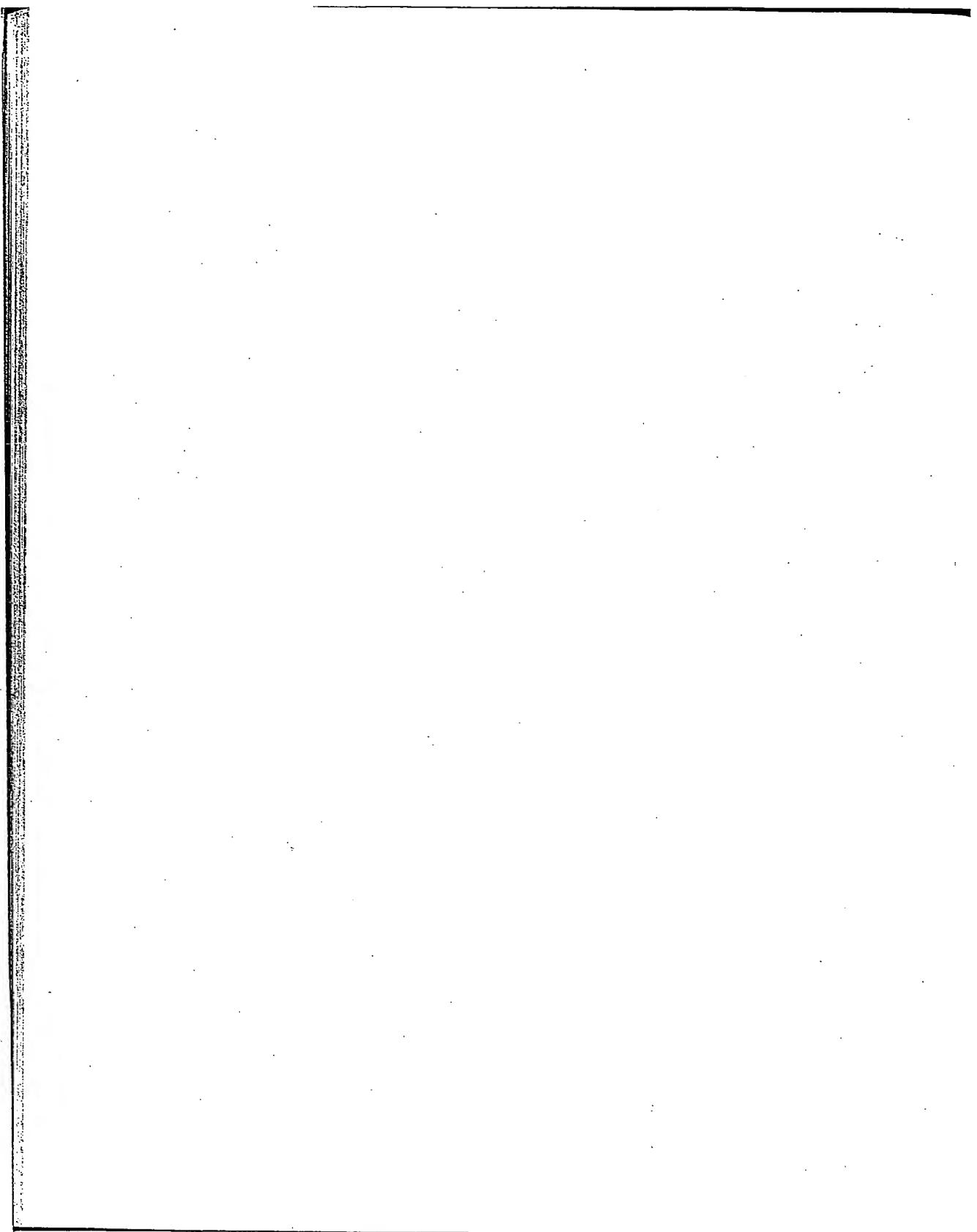
- Select the Chemical Symbol tool.
- Hold down the Shift key and point at a Chemical Symbol.

A highlight box appears.

- Drag the highlight box on the chemical symbol.

The symbols are rotated around the same end from which they were originally drawn. For instance, the radical cation symbol is rotated and resized from the charge. As you rotate symbols, the angle that one of the ends of a symbol makes with the X axis is shown in the Message area.

You can also rotate many of the symbols using the Selection tool by dragging the Rotation handle on the Selection Rectangle. The charge and the radical symbols cannot be rotated. The rotation occurs around the center of the object as defined by the Selection rectangle. Equal rotations performed by the Selection tool and the Chemical Symbols tool will result in a different final placement of the object rotated. For general information about rotating and resizing, see "Rotating Objects" in *Chapter 7, Working with Selections*.



Chapter 6, Drawing Arrows, Arcs and Other Shapes

This chapter discusses four tools that you can use to add different kinds of shapes to your documents. These tools include the Arrow tool for drawing arrows, the Arc tool for drawing arcs, the Drawing Elements tool for drawing boxes, circles and brackets, and the Pen tool for drawing freehand shapes.

The Arrow, Arc and Drawing Elements tools each contain a palette from which you can choose from different types of that tool. Once you choose a tool from the palette, that tool can be used without choosing from the palette again.

To select a tool and use its default object:

- Click the tool's icon to select it.

To choose a different object from the palette:

- Point to the tool's icon and hold down the mouse button.

The palette appears.

- Drag to select an object from the palette.
- Release the mouse button over the object you want to select.

The new object becomes the default used for that tool whenever you select the tools icon from this point forward, until you make another selection from the palette.

The remainder of this chapter will step through each of the tools individually.

THE ARROW TOOL

The Arrow tool is used for adding arrows to show conversion of reactants to products as well as indicating electron flow (you can also use the Pen tool, discussed later in this chapter, to make customized arrows).

Figure 6-1 Arrow tool

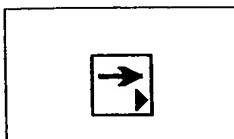
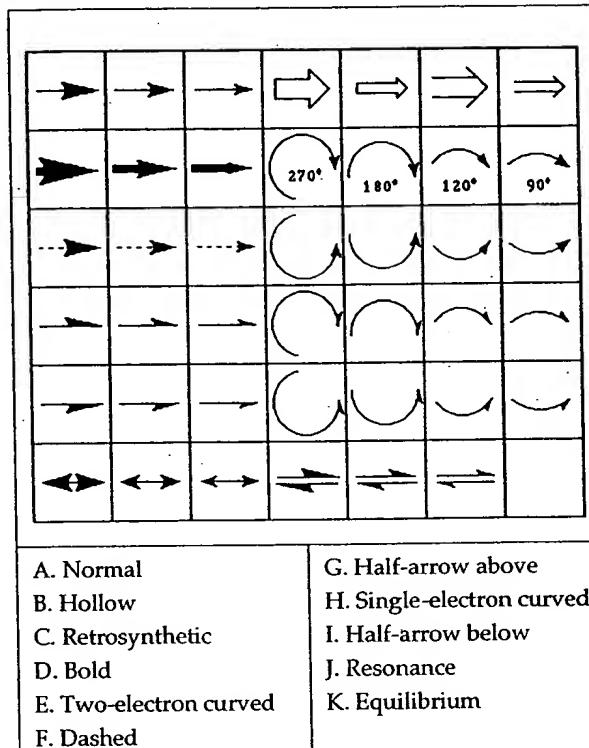


Figure 6-2 Types of arrows in the Arrow Tool palette



Drawing an Arrow

- Select the Arrow tool.
- Point in the document where you want the end of the arrow to appear.
- Drag to where you want the arrow head to be.

Editing an Arrow

To lengthen, shorten or rotate an arrow:

- **Select the Arrow tool.**
- **Hold down the Shift key and point to the head of the arrow.**

A highlight box appears over the head of the arrow.

- **Drag the arrowhead.**

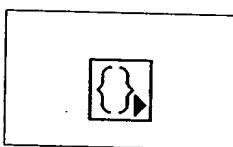
The arrow is resized and rotated relative to its end. As you drag, the change in length and the angle the arrowhead makes with the X axis appear in the Message area.

You can also resize and rotate an arrow using the Selection tool by dragging the Resize or Rotation handle on the Selection rectangle. The Message area indicates the percentage enlarged or reduced when you drag the Resize handle and the number of degrees rotated when you drag the Rotation handle. The resize or rotation occurs around the center of the Selection rectangle. Equal rotation or resize operations performed by the Selection tool and the Arrow tool will result in a different final placement of the object. You cannot change the aspect ratio of arrows. See "Rotating Objects" and "Resizing Objects" in *Chapter 7, Working with Selections*, for general information.

THE DRAWING ELEMENTS TOOL

The drawing elements tool provides a variety of shapes that can add to your drawing.

Figure 6-3 The Drawing Elements tool



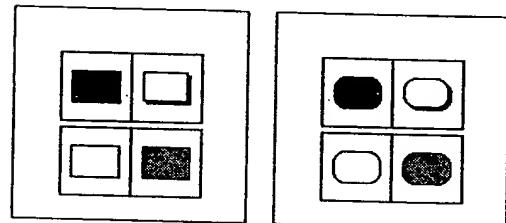
Several Drawing Element types are available with different fill patterns: hollow (no fill pattern), gray and black.

Gray Drawing Element types appear with grayscale shading on color and grayscale monitors and print with grayscale shading from PostScript printers when the Color/Grayscale option is selected in the Print dialog box.

Related groups of Drawing Element types are discussed below. While you draw any of the drawing element types, the length and angle relative to the X axis appears in the Message area.

Boxes

Figure 6-4 Boxes

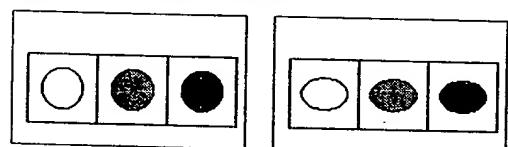


To draw a box:

- **Select a box tool.**
- **Point where you want a corner of the box to be located.**
- **Drag from one corner of the box diagonally to the opposite corner.**

Circles and Ovals

Figure 6-5 Circles and ovals



To draw a circle or oval:

- **Select a circle or oval tool.**
- **Point where you want the center of the circle to be located.**

- Drag outward from the center.

NOTE: to make other styles of circles, such as a dashed circle, you can use the pen tool with dashed style. See "Pen Tool" later in this chapter.

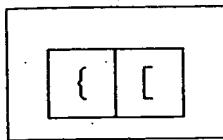
Single Brackets

To draw a single bracket:

- Select a single bracket tool.
- Point where you want the bracket to start.
- Drag from one end of the bracket to the other end.

A single bracket can be drawn in any orientation.

Figure 6-6 Single brackets



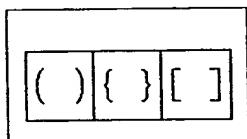
Paired Brackets

To draw a paired bracket:

- Select a paired bracket tool.
- Point where you want a corner of the bracket to be located.
- Drag from one corner of the box diagonally to the opposite corner.

Paired brackets can only be placed in a vertical orientation. Their position is defined by a rectangle or box.

Figure 6-7 Paired bracket



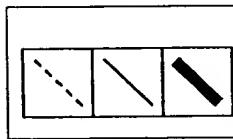
Lines

Lines drawn with the line tool differ in two significant ways from bonds drawn with the bond tools: they are not counted in chemical interpretation of the drawing, and they do not "drop out" when they cross one another.

To draw a line:

- Select a line tool.
- Point where you want the line to start.
- Drag from one end of the line to the other end.

Figure 6-8 Dashed and solid lines

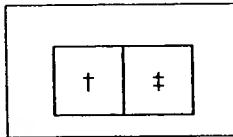


Daggers

To draw a dagger:

- Select a dagger tool.
- Point where you want the symbol to be located.
- Click to deposit the dagger.

Figure 6-9 Daggers



NOTE: Drawing elements, such as brackets, are not actually part of the structure they are drawn near, and are not selected if you double-click on a bond, atom or atom label with the Selection tool. To group drawing elements with a structure, use the Group command in the Object menu. To learn more about grouping, see "Grouping" in Chapter 7, Working with Selections.

Editing Drawing Elements

To resize or rotate a drawing element:

- Select the Drawing Element tool.
- Hold down the Shift key and point to an end or edge of a drawing element.

A highlight box appears.

- Drag the object to the new size or orientation (not valid for boxes and closed brackets)

The drawing element is resized or rotated from the same point that it was originally drawn. For instance, a shadowed box is resized from the corner where the shaded edges meet. The length of the drawing element and the angle it makes with the X axis appears in the Message area. Boxes and paired brackets cannot be rotated.

NOTE: The size of the dagger symbol is proportional to the Atom Label font size specified in the Text Settings dialog box.

You can also resize and rotate many of the drawing elements using the Selection tool by dragging the Resize or Rotation handle on the Selection rectangle. You cannot rotate Dagger symbols. The percentage enlarged or reduced when you drag the Resize handle and the number of degrees the object rotates when you drag the Rotation handle appears in the Message area. The resize or rotation occurs around the center defined by the Selection rectangle. Equal rotation or resize operations performed by the Selection tool and the Drawing Elements tool will result in a different final placement of the object.

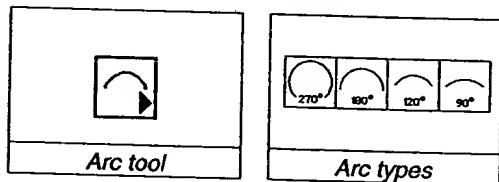
Distorting circles and ovals (Alt+dragging (or Command+dragging) the Resize handle) converts these objects into an equivalent closed curve. Distorting gray shaded circles and ovals converts these objects to solid filled curves where the fill color is the same as the color of the curve. You can also distort boxes and closed brackets. The remaining Drawing Element types cannot be distorted. See "Rotating Objects" and "Resizing Objects" in Chapter 7, Working with Selections.

Closed brackets and boxes cannot be rotated in the usual sense; however, when a box or closed bracket is rotated along with object(s) within its borders, the area of the box or closed bracket increases to accommodate the rotation of the contained objects.

THE ARC TOOL

The Arc tool is used to draw arcs of different angles: 90°, 120°, 180°, and 270°.

Figure 6-10 The Arc tool and palette



NOTE: On a small monitor, such as on the SE/30, the Arc types described in this chapter are located in the Drawing Elements palette discussed earlier in this chapter.

Drawing an Arc

To draw an arc:

- Select an arc tool.
- Drag from the left edge of the arc to the clockwise end of the arc in a document window.

While you draw an arc, the length between the ends, and the angle the clockwise end makes with the X axis appears in the Message area.

Editing an Arc

To resize or rotate an arc using the Arc tool:

- Select the Arc tool.
- Hold down the Shift key and point to the clockwise end of the arc.

A highlight box appears.

- Drag the clockwise end of the arc.

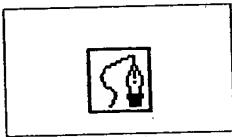
The arc is resized and rotated relative to the first end from which it was drawn. The distance between the ends of the arc and the angle the clockwise end makes with the X axis appears in the Message area.

You can also resize and rotate an arc using the Selection tool by dragging the Resize or Rotation handle on the Selection rectangle. The Message area indicates the percentage enlarged or reduced when you drag the Resize handle and the number of degrees rotated when you drag the Rotation handle. The resize or rotation occurs around the center defined by the Selection rectangle. Equal rotation or resize operations performed by the Selection tool and the Arc tool will result in a different final placement of the object. You cannot distort arcs. See "Rotating Objects" and "Objects" in Chapter 7, *Working with Selections*, for general information.

THE PEN TOOL

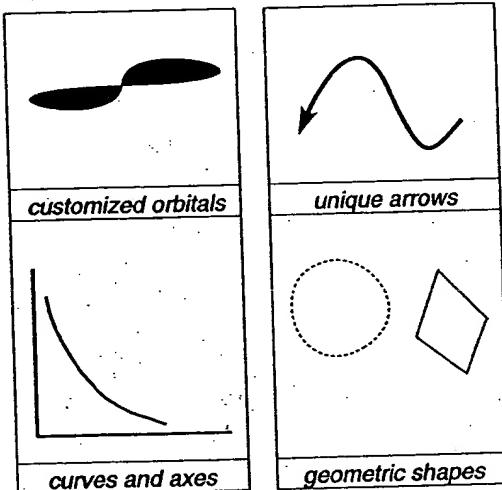
Using the Pen tool, you can draw shapes that are not provided in the arrow, orbital or drawing elements palettes. For instance, you can draw irregularly shaped arrows, curves depicting graphs or reaction coordinate diagrams, as well as any other irregularly-shaped solids.

Figure 6-11 The Pen tool



Below (Figure 6-12) are some examples of shapes that you can draw using the Pen tool.

Figure 6-12 Shapes drawn using the Pen tool



To select the Pen tool:

- Click the Pen tool icon in the Tools palette.

Shortcut:

To toggle between the Selection tool and the Pen tool:

- Press **Ctrl+Alt+Tab** (Windows) or **Command+Tab** (Macintosh) or select the Selection tool.

The last drawn curve and the selection tool are selected.

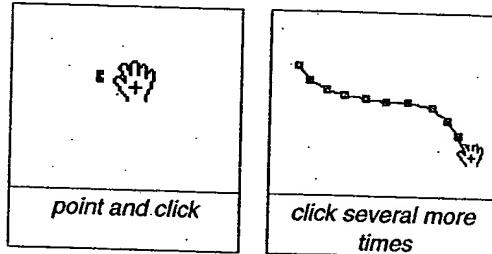
Drawing Segments by Clicking

The easiest way to draw shapes with the pen tool is to click repeatedly in an outline of the shape you want.

- Select the Pen tool.
- Point to where you want the beginning of the curve to appear.

- Click to deposit an endpoint.
- Move the cursor and click again to add a second endpoint. Continue until you have the curve you want.
- Press the Escape key or click another tool.

Figure 6-13 Shapes drawn by clicking with the Pen tool



NOTE: you might want to work in a magnified view so you can place the fewest strategically placed control points for obtaining the smoothest curve.

Drawing Bézier Curves by Dragging

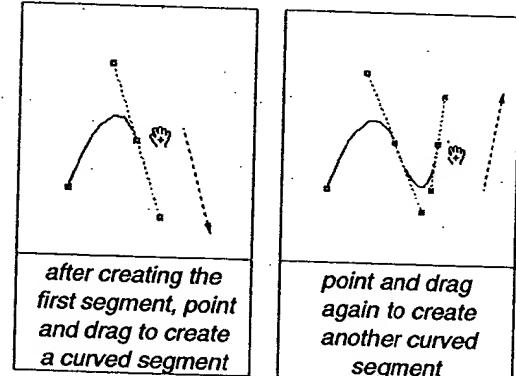
A second way to draw curves with the pen tool is to click and drag repeatedly to create curved segments.

- Select the Pen tool.
- Point to where you want the beginning of the curve to appear.
- Click and drag in the direction of the curve.
- Move the cursor to another position.
- Hold down the mouse button and drag to create an arc.
- Press the Escape key to get out of the drawing mode of the curve tool.

Once you hold down the mouse button, another endpoint is established. Dragging creates the curve portion of the segment.

Notice that an additional line appears tangentially to the curve. This is the direction line that you can use to control the "curviness" of the segment.

Figure 6-14 Creating a curve with the Pen tool



There are two kinds of control points that define the curve of a Bézier curve: endpoint controls and direction controls. The curve will pass through each endpoint control in turn, and its path from one endpoint to the next is determined by the direction controls.

Editing a Curve

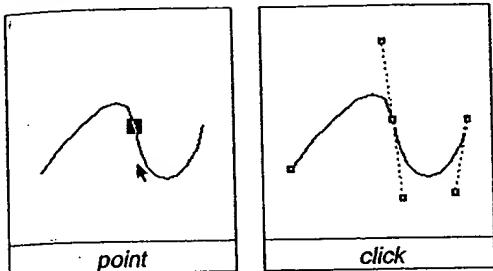
To select an existing curve:

- Select the Pen tool.
- Point at the center of the curve.

A highlight box will appear when you are positioned correctly.

- Point at the center of the curve.

Figure 6-15 Selecting a curve with the Pen tool

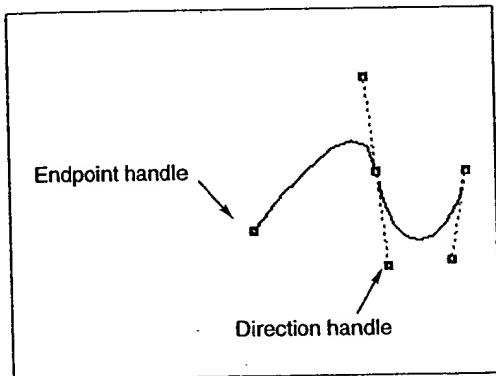


A highlight box appears.

- Click the highlight box to select the curve.

The components of the curve appear. The components of the curve are shown in Figure 6-16.

Figure 6-16 Appearance of handles on a selected curve

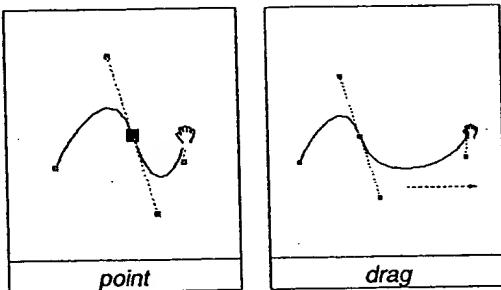


Changing Shape

The control points that appear as you draw a curve allow you to change the size and curve of a curve segment.

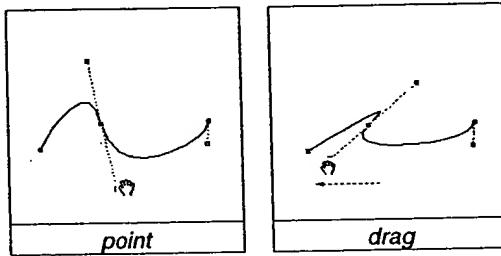
Each point that touches the curve is an endpoint handle. Dragging an endpoint handle increases or decreases the breadth of the curve.

Figure 6-17 Changing a curve by dragging an endpoint handle



The lines that pierce each point are the direction lines for the segment. The direction line controls the direction of the curved portion of the segment.

Figure 6-18 Changing curve by dragging a direction handle



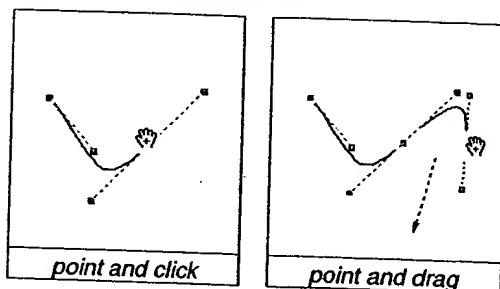
Adding a Segment

To extend an existing curve:

- Select the Pen tool, and click the existing curve you want to edit to select it.

The components of the curve appear.

Figure 6-19 Adding segments



- Point to the Endpoint handle of a curve until the cursor appears as a hand.
- Ctrl+click (Windows) or Option+click (Macintosh) the endpoint.

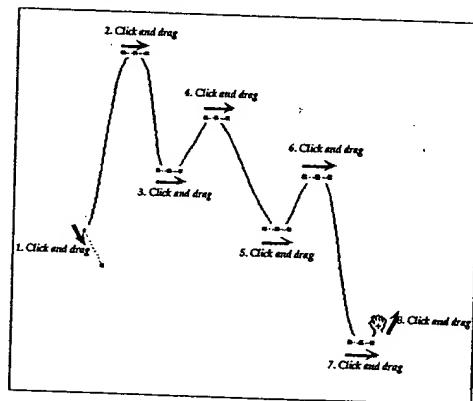
The cursor now appears as a hand with a “+” sign inside, and note that the endpoint now appears has the components of a middle segment, i.e., it now has two tangent control lines. The Pen tool is in drawing mode.

- Click and drag in the window to connect more segments to your curve.

To exit the drawing mode:

- Press the escape key or click the Pen tool or any other tool, or double-click.

Figure 6-20 Using the Pen tool to draw reaction mechanism diagrams



Deleting a Segment

To delete a curve segment: (You should be in the edit mode of the Pen tool, i.e., the cursor should appear as a Crosshair.)

- Ctrl+Shift+click (Windows) or Option+Shift+click (Macintosh) the control point where you want to delete a curve segment. (The cursor should appear as the Eraser tool before you click.)

You can also delete entire curves using the Selection tool and the Eraser tool.

Applying a Style

To apply a style to a curve:

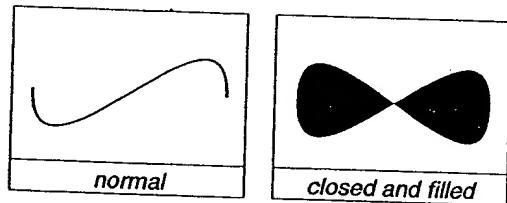
- Select a curve using either the Pen tool or the Selection tool.
- From the Curves menu, choose a style.

All curves are drawn with the last curve styles chosen until you change the selections. Certain styles are mutually exclusive. For instance, if you choose Closed, you cannot also choose Arrow at Start.

To remove all styles from a curve:

- From the Curves menu, choose Plain.

Figure 6-21 Shape with and without closed and filled style



Chapter 7, Working with Selections

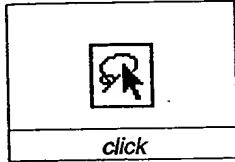
A large portion of the editing in ChemDraw is performed using the Selection tool. With the Selection tool you can select individual objects and groups of objects. Once objects are selected, you can duplicate, move, resize, rotate or delete them. This chapter describes these and other editing operations you can accomplish with the Selection tool.

USING THE SELECTION TOOL

To select the Selection tool:

- Click the Selection Tool icon in the Tools palette.

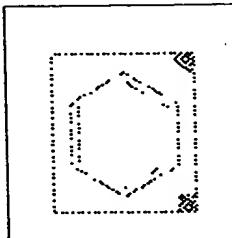
Figure 7-1 The Selection Tool



The Selection tool is highlighted, indicating that it is the currently selected tool. In addition, the last object, curve, caption or atom label drawn appears within a shimmering rectangle called the Selection rectangle, indicating that it is selected and can be manipulated.

When you select the selection tool the last object drawn is automatically selected. You can deselect this object, add to or remove from the selection using the selection techniques discussed in this chapter.

Figure 7-2 A Selection rectangle



Shortcut

To quickly switch to the Selection tool from some other tool:

- Press **Ctrl+Alt+Tab** (Windows) or **Command+Tab** (Macintosh).

The Selection tool and the last drawn object are selected.

To switch from the Selection tool to the last drawing tool used:

- Press **Ctrl+Alt+Tab** (Windows) or **Command+Tab** (Macintosh).

Selecting Objects by Clicking

To select an object by clicking:

- Select the Selection tool.
- Point to an object in a document window.

A highlight box appears over the objects that will be selected when you click. If you point at a bond, the highlight box appears over the length of the bond. If you point to an unlabeled atom, each of the connecting bonds will have a highlight box, indicating that they will be selected when you click.

- Click a bond, an unlabeled atom or other object.

The selected object appears within the Selection Rectangle and the cursor changes to a hand.

Figure 7-3 Selecting a bond

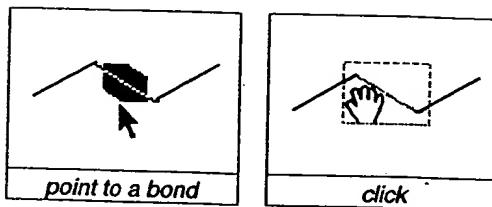
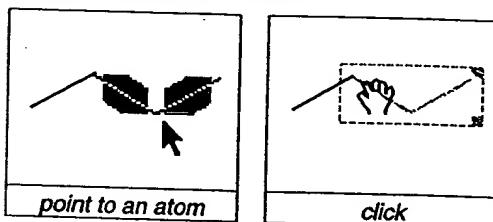


Figure 7-4 Selecting several bonds



NOTE: If the bond or other object is part of a group you can still select it as an individual object. For more details about grouping objects see "Grouping" later in this chapter.

Preferences Guide Tolerance

The size of the highlight box (and how close you must get to an object to activate highlight boxes) is controlled by the measurement in the box labeled "Tolerance" in the Preferences dialog box. The standard setting for the Tolerance is 5 pixels. This means, for instance, that the highlight box appears on bonds if the pointer is located 5 pixels or less from any point on the bond.

To change the Tolerance:

- From the File menu, choose Preferences.
- Click the up or down Tolerance control arrow to increase or decrease the tolerance.

This change affects all documents.

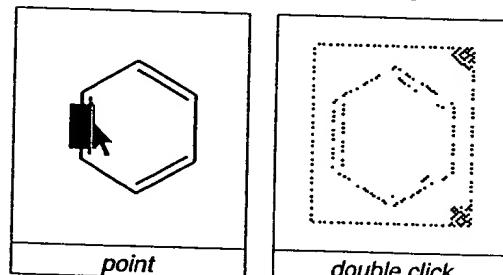
Selecting Entire Structures

To select an entire chemical structure:

- Double-click a bond or atom within the structure.

The entire chemical structure is selected. If the chemical structure or other object is part of a group, the entire group is selected. Also see "Grouping" later in this chapter.

Figure 7-5 Selecting by double-clicking



Selecting Objects with the Lasso

You can use the Lasso to encircle irregular areas in a document window, such as part of a chemical structure.

To select objects using the Lasso:

- Select the Selection tool.
- Press the mouse button while the pointer is not over any object.
- Drag around a portion of a chemical structure or other object.

As you drag around the object(s), a line appears which defines the Selection area. Only bonds, structures or other objects that are entirely enclosed in the Selection area will be selected. The end points of the Lasso are automatically connected when you release the mouse button.

Figure 7-6 Selecting parts of a structure using the lasso

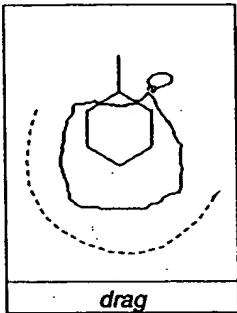
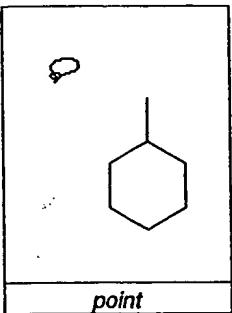
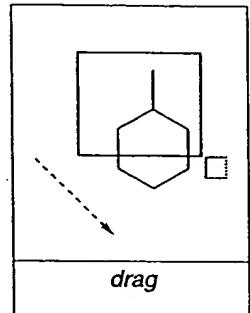
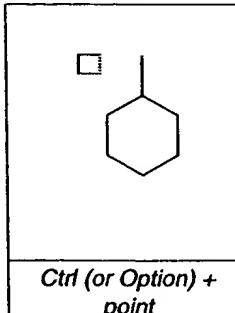


Figure 7-7 Selecting parts of a structure using the Marquee



Selecting Objects with the Marquee

You can use the Marquee to select objects and structures within a rectangular area.

To select objects using the Marquee:

- **Select the Selection tool.**
- **Hold down the Ctrl (Windows) or Option (Macintosh) key while the pointer is not over any object.**

The pointer becomes a Marquee.

- **Drag diagonally across the chemical structure(s) or other object(s).**

As you drag, a rectangle appears which defines the Selection area. Bonds and other objects are selected only if they are entirely within this area. The Marquee is useful for selecting several objects at once as long as they can be surrounded by a rectangle.

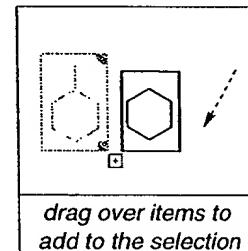
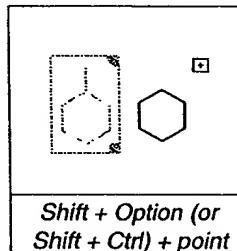
Adding to the Selection

To make multiple selections or add more objects to the selection:

- **Hold down the Shift key and select several other objects.**

Objects can be added to the Selection by clicking, double-clicking or by using the Lasso.

Figure 7-8 Adding to a selection using the Marquee mode of the Selection tool



Removing Objects from the Selection

To remove an object from the selection:

- Hold down the Shift key and select an object contained within the Selection rectangle by clicking, double-clicking, or Lassoing.

The object is removed from the selection.

NOTE: Objects may appear within the borders of the Selection rectangle, but not be selected. Only objects that are shimmering are selected.

Selecting All Objects

To select all objects within a document window:

- From the Edit menu, choose Select All.

Deselecting All Objects

To deselect all selected objects:

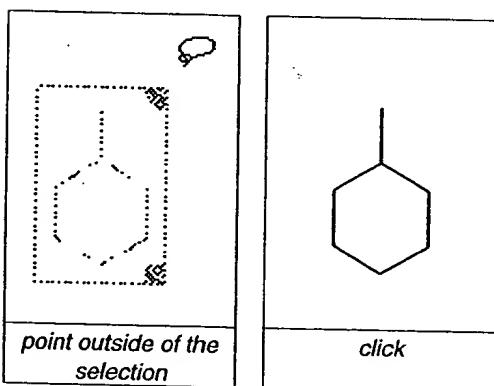
- Click in any empty area in a document window that is outside the Selection rectangle.

Alternatively:

- Press the Escape key.

All selected objects are deselected. You can also deselect all selected objects by selecting a different tool or by selecting another object without holding down the Shift key.

Figure 7-9 Deselecting an object



Deleting Objects

You can delete selected objects using the Delete key, the Clear command, or the Eraser tool.

Delete key

To delete object(s) using the Delete key (or the Backspace key):

- Select the object(s) you want to delete.
- Press the Delete key.

Clear Command

To delete object(s) using the Clear command:

- Select the object(s) you want to delete.
- From the Edit menu, choose Clear.

The Eraser Tool

With the Eraser tool you can delete objects selectively. For instance, you can reduce the bond order of a multiple bond, or erase a single bond. Below are the general rules followed by the Eraser tool:

- ⇒ Clicking a labeled atom removes the label.
- ⇒ Clicking an unlabeled atom removes the atom and all adjacent bonds.

To select the Eraser tool:

- Click the Eraser tool icon in the Tools palette.

Figure 7-10 The Eraser Tool



To erase a bond:

- Click a single, double or triple bond.

The bond order is reduced by one.

Figure 7-11 Erasing one bond of a double bond

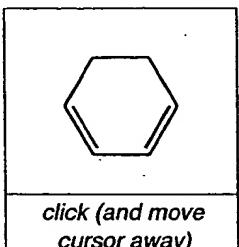
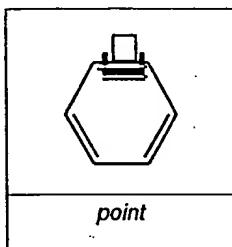
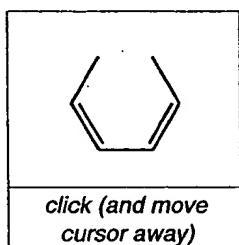
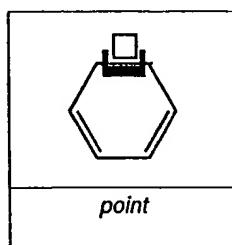


Figure 7-12 Clicking a single bond with the Eraser tool

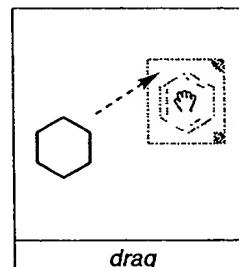
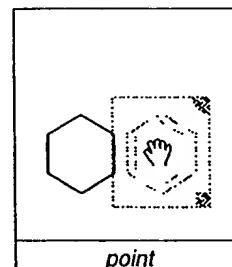


MOVING OBJECTS

To move an object:

- Select the object(s) using the Selection tool.
- Point within the border of the Selection rectangle.
- Drag the object(s).

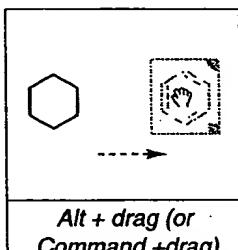
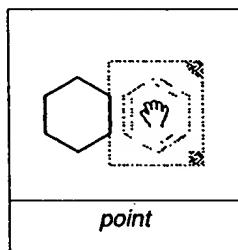
Figure 7-13 Moving a selected object



To constrain the movement to the horizontal or vertical direction:

- Alt+drag (Windows) or Command+drag (Macintosh) the selected object(s).

Figure 7-14 Moving and constraining a selected object



To move selected objects a small distance using the Arrow keys available on many keyboards:

- Press an arrow key while object(s) are selected.

The selected object(s) move 1 point (1/72 inch, 0.035 cm) in that arrow's direction.

To move in a larger increment, for example, to the right:

- Press Ctrl+Right Arrow (Windows) or Option+Right Arrow (Macintosh)

The selected objects move 10 points (10/72 inch, 0.35 cm) in that arrow's direction. These small incremental movements are often useful for aligning objects.

NOTE: See Chapter 12, *Working with Page Layout*, for more information about aligning objects.

Using the Clipboard

To remove the objects contained in the Selection rectangle for later repositioning in the current document window, or for transferring to another ChemDraw document or other type of document:

- Select the object(s) using the Selection tool.

- From the Edit menu, choose Cut.

The object is transferred to the Clipboard and deleted from a document window. You can transfer the copy on the Clipboard to another position in the same document, another *ChemDraw* document or a different type of document.

To paste a copy of the contents of the Clipboard into a document window:

- Select the Selection tool.
- From the Edit menu, choose Paste.

NOTE: For important information about transferring *ChemDraw* pictures to other types of documents see "Autoscaling" in Chapter 13, *Sharing Information*.

You can also use Drag and Drop to move selections between *ChemDraw* documents. See "Drag and Drop" in Chapter 13, *Sharing Information*, for additional information.

Moving Atoms

You can move the atoms within a chemical structure using the Selection tool.

To move a single atom:

- Point to an atom using the Selection tool.
- Drag the atom.

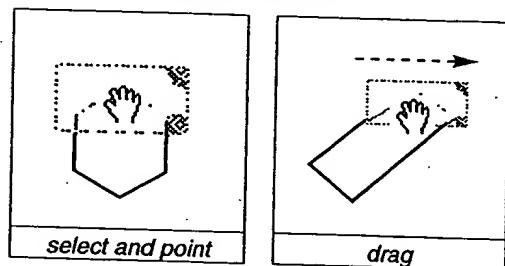
The bonds connected to the atom stretch as it is dragged. If you drag an atom on top of an adjacent atom, the atom and the bond between the atoms disappear. This is useful for converting 6-membered rings into 5-membered rings.

To move multiple atoms:

- Select only the bonds that have atoms on both ends that you want to move.

The unselected bonds that are attached to the selected atoms will be stretched.

Figure 7-15 Dragging a selection



NOTE: You can also move atoms using the bond tool that was used to draw the atom. See "Moving Atoms" in Chapter 3, *Drawing Chemical Structures*.

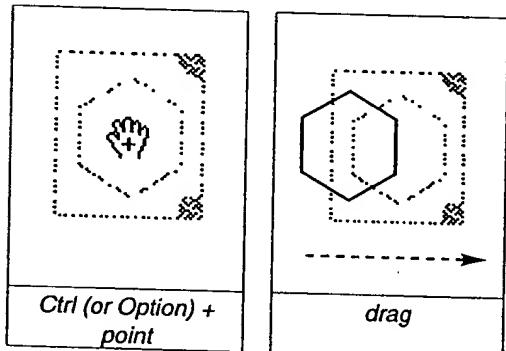
DUPLICATING OBJECTS

To duplicate objects with the Selection tool:

- Select the Selection tool.
- Select the object(s).
- Ctrl+drag (Windows) or Option+drag (Macintosh) to create a copy and position it.

A copy of the selected objects is moved to the new position.

Figure 7-16 Duplicating a selection



To duplicate the selected objects and constrain the positioning of the copy to the same horizontal or vertical position as the original objects:

- Select the Selection tool.
- Select the object(s).
- Ctrl+Alt+drag (Windows) or Option+Command+drag (Macintosh) to create a copy and position it.

To place a copy of an object on the Clipboard:

- Select the object(s) using the Selection tool.
- From the Edit menu, choose Copy.

A copy of the object is placed on the Clipboard. Using the Paste command, you can transfer the copy in the Clipboard to the current document, another ChemDraw document, or a different document type.

NOTE: For important information about transferring ChemDraw pictures, see "Autoscaling" in Chapter 13, Sharing Information.

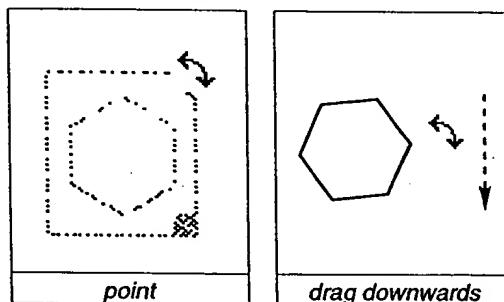
ROTATING OBJECTS

To rotate object(s):

- Select the object(s) to rotate using the Selection tool.
- Drag the Rotation handle clockwise or counterclockwise.

The Rotation handle is located in the upper-right corner of the Selection rectangle:

Figure 7-17 Rotating a selection



As you rotate, the magnitude of the rotation around the center of the Selection rectangle appears in the Message area.

NOTE: Captions and atom labels that contain multiple colors will change to the foreground color when rotated. However, all colors contained in the captions are printed.

To rotate objects, but not atom labels:

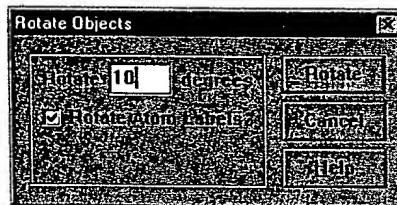
- Hold down the Ctrl key (Windows) or the Option key (Macintosh) and drag the Rotation handle.

To rotate the selected object(s) a specified number of degrees:

- From the Object menu, choose Rotate.
- Or, double-click the Rotation handle.

The Rotation dialog box appears.

Figure 7-18 Rotate dialog box



- Enter a positive whole number for a clockwise rotation or a negative whole number for counterclockwise rotation.
- Click the Rotate button.

Objects are rotated around the center of the Selection rectangle.

To perform another rotation of exactly the same magnitude on any object in the document window, immediately after performing a rotation:

- Select the other object(s) to rotate.
- From the Edit menu, choose Repeat Rotate.

REFLECTING OBJECTS THROUGH PLANES

You can reflect structures through planes perpendicular to the X or Y axis using the Selection tool. Used in conjunction with duplicating, you can create mirror images of chemical structures for representing racemic mixtures, and with a small amount of editing, other stereoisomers as well.

To reflect an object through a plane perpendicular to the Y axis:

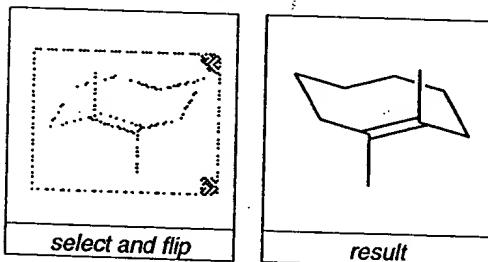
- Select the object(s) to reflect.
- From the Object menu, choose Flip Vertical.

To reflect an object through a plane perpendicular to the X axis:

- Select the object(s) to reflect.
- From the Object menu, choose Flip Horizontal.

Atom labels and captions do not flip along with the object.

Figure 7-19 Reflecting an object horizontally by choosing Flip Horizontal



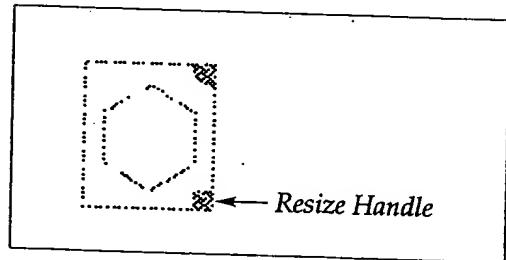
RESIZING OBJECTS

To resize an object or collection of objects:

- Select the object(s) to resize.
- Drag the Resize handle.

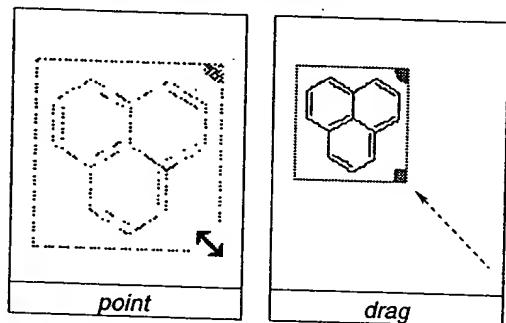
The Resize handle is located in the lower right corner of the Selection rectangle.

Figure 7-20 Resize handle



As you resize the selected object(s), the percentage you have enlarged or reduced it from the original size is shown in the Message area.

Figure 7-21 Resizing a selection



NOTE: If all objects in the document window are part of the selection you are resizing, a message appears after you resize that asks whether you want to change the document settings for that document. If you choose to do so, all subsequent bonds, atom labels and captions (depending on what is in the selection) will be drawn using these new settings.

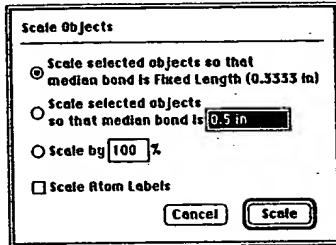
The Scale Dialog Box

You can also resize objects with the Scale command:

- Select the object(s) to scale.
- From the Object menu, choose Scale,
- Or, double-click the Resize handle.

The Scale Dialog Box appears (Figure 7-22).

Figure 7-22 Scale dialog box



The first two options in the Scale dialog box are used to scale all selected objects so that the median selected bond has a specified length based on the following scale factor:

Figure 7-23 Scale factor equation

$$\text{scale factor} = \frac{\text{new median bond length}}{\text{current median bond length}}$$

To scale bonds in the selected objects so that the Fixed Length indicated in the Drawing Settings dialog box is used as the new median bond length:

- Select the top option/radio button.

The fixed length presently in the Drawing Settings dialog is shown in parentheses at the end of the line for this button.

- Click the Scale button.

To scale the bonds to a new fixed length that you specify:

- Select the middle option/radio button.
- Type the new median bond length in the box to the right of the button.

The current median bond length for the selection is shown in the highlighted text box when the dialog box initially appears.

- Click the Scale button.

To scale object(s) by a percentage:

- Select the bottom option/radio button.
- Type the percentage in the box to the right of the button.
- Click the Scale button.

This last option is the only one available when the selection does not contain any atoms or bonds.

Distorting a Selection

In most cases, when you resize an object, the aspect ratio of the object (the ratio of the object's height to its width) does not change. However, it is possible to change the aspect ratio (distort) of certain objects including chemical structures, circles, boxes, and ovals.

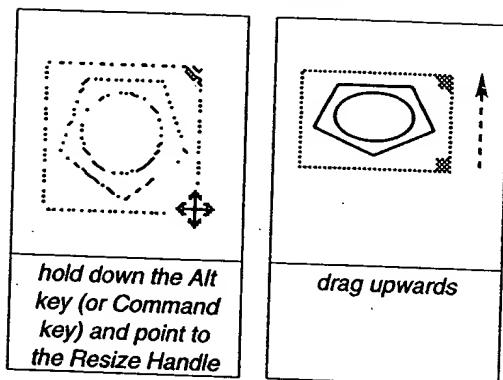
To distort an object in the horizontal or vertical direction:

- Select the object and Alt+drag (Windows) or Command+drag (Macintosh) the Resize handle.

The Alt key (Windows) or Command key (Macintosh) modifies the resize operation so that you can distort objects along the X or Y axis.

- Drag the Resize handle.

Figure 7-24 Distorting a selection



JOINING OBJECTS

Use the Join command in the Object menu to fuse two chemical structures together. Once structures are joined they can be easily selected by double-clicking.

To join chemical structures along the length of a bond:

- Position the structures that you want to join so that the bonds you want to join are nearly overlapping (within tolerance).

Objects to be joined must be positioned close enough to be within the Tolerance setting specified in the Drawing Settings dialog box. Otherwise, the Join command will be inactive.

- Select the chemical structures to join.
- From the Object menu, choose Join.

To join chemical structures at one atom to create a spiro-linkage:

- Select both chemical structures.
- Position the two chemical structures so that two atoms nearly overlap.
- From the Object menu, choose Join.

NOTE: When you join two differently colored bonds or atom labels, the color of the frontmost object becomes the color of the resulting joined object. See Chapter 12, Working with Page Layout, for more information about front to back ordering of objects.

NOTE: When you join two atoms that are labeled, the frontmost atom label becomes the atom label of the resulting atom.

Figure 7-25 Fusing bonds

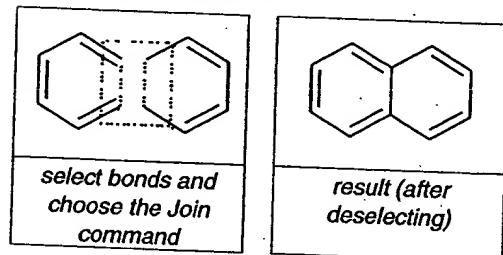
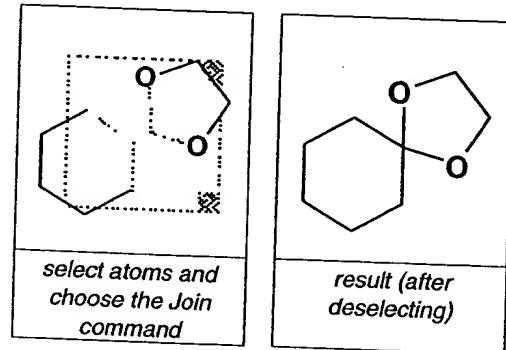


Figure 7-26 Fusing atoms



Preferences Guide

Tolerance

The maximum distance required between two atoms for joining to occur is controlled by the Tolerance setting in the Preferences dialog box. The standard setting for the Tolerance is 5 pixels. This means that two atoms will be joined if they are within 5 pixels of each other when you choose the Join command.

To change the Tolerance:

- From the File menu, choose Preferences.
- Adjust the number of pixels by clicking the up or down Tolerance spin button.

This change affects all documents.

GROUPING

It is often convenient to group a number of objects drawn separately into a single group. All objects contained in a group can be selected by double-clicking with the Selection tool. Objects within a group can be selected individually and manipulated while still remaining part of the group. Grouping does not lock the position or orientation of objects; grouping only creates an association between objects so they can be easily selected.

Grouped objects also maintain their relative positions when they are centered on the page, aligned or distributed.

Atoms and bonds making up a single chemical structure are always grouped. If you group part of a structure with other objects, the resulting group will contain the entire structure. If you add atoms or bonds to a grouped structure, the new atoms and bonds will be part of the group.

NOTE: Only one level of grouping is provided. For instance, if you create two grouped objects, group these groups and then ungroup them, you return to the individual objects — not the groups.

Group

To group several objects:

- Select the objects to group using the Selection tool.
- From the Object menu, choose Group.

To select a group:

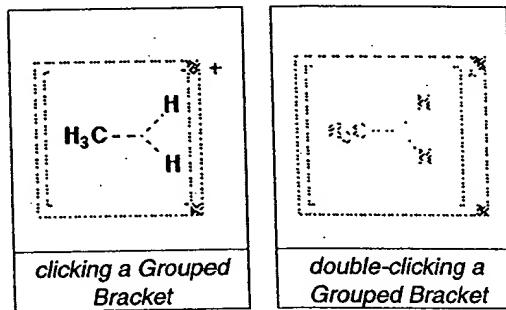
- Double-click an object within the group using the Selection tool.

To select an individual object within a group:

- Click the object using the Selection tool.

The object is selected, not the group.

Figure 7-27 Clicking and double-clicking grouped brackets

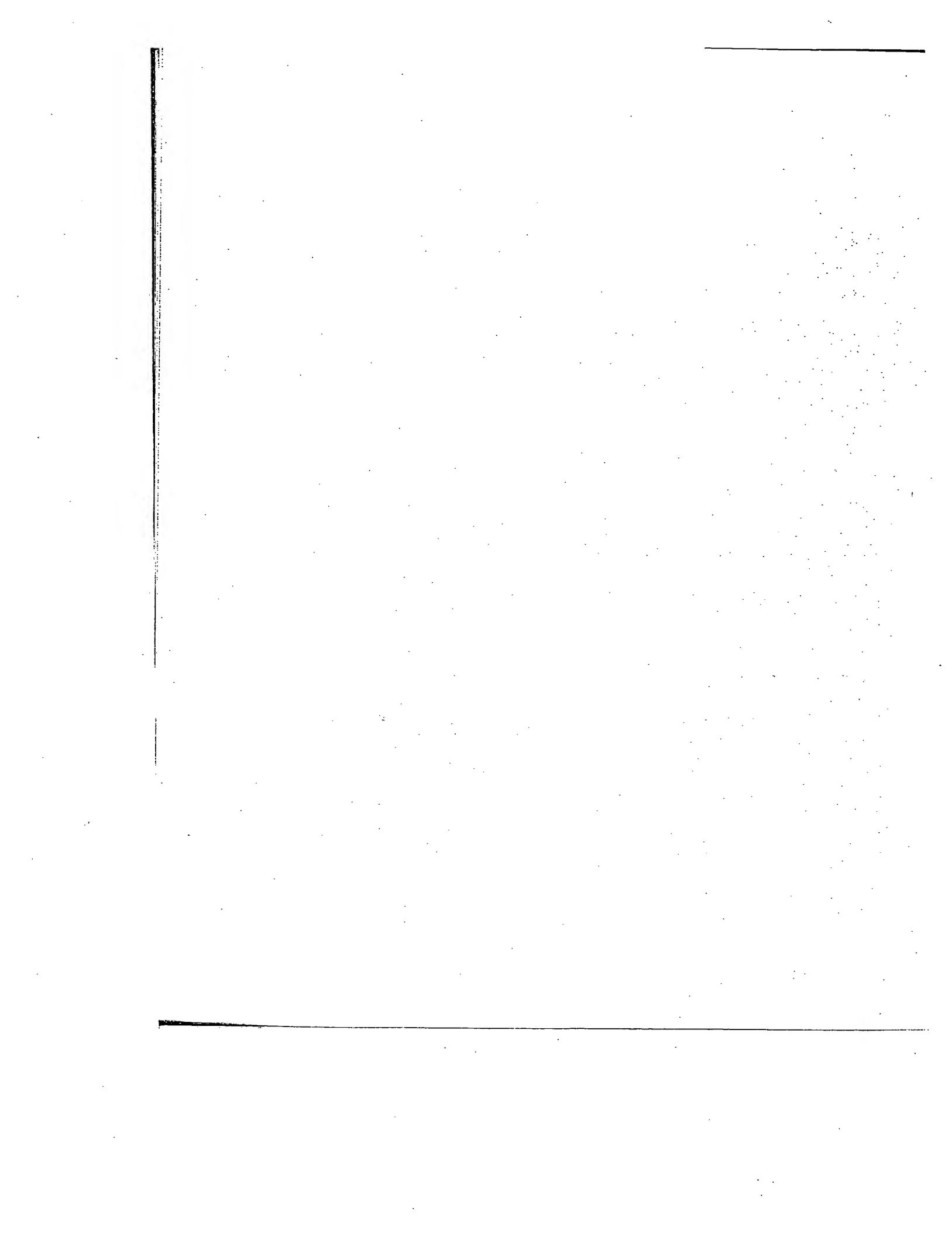


Ungroup

To ungroup objects that are grouped:

- Double-click a group using the Selection tool.
- From the Object menu, choose Ungroup.

All the objects previously grouped become individual objects.



Chapter 8, Advanced Drawing Techniques

This chapter discusses the advanced drawing features available in *ChemDraw*. These advanced features provide alternative ways to label atoms by using HotKeys and abbreviated forms of functional groups called "Nicknames." In addition, this chapter discusses advanced drawing techniques for adding bonds to specific characters in atom labels, expanding nicknames, and creating bonds whose attachment is not explicitly defined.

USING HOTKEYS TO LABEL ATOMS

Use *ChemDraw* HotKeys to quickly label atoms and apply atom properties. The file, "hotkeys.txt" (Windows) or "ChemDraw HotKeys" (Macintosh), located in your cd_items directory (Windows) or *ChemDraw* Folder (Macintosh), contains the HotKeys provided with *ChemDraw*. You can add or change HotKeys by editing the file in a text editor, such as Notepad, TeachText, or SimpleText. See the section "Creating HotKeys" to learn how.

There are several ways to use a HotKey to label an atom. Following are descriptions of each method.

Method 1: labeling the last atom drawn

- Draw a bond.
- Press a HotKey.

The last atom drawn is labeled. Each time you draw a bond, the last atom drawn will be the HotKey atom.

Method 2: labeling an atom at which you point

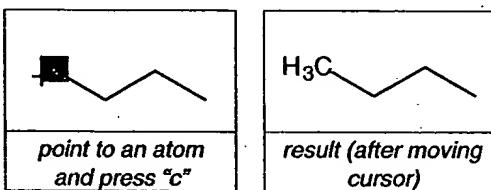
- Position the pointer over an atom.

A highlight box appears over the atom when you are using a bond tool or the Text tool.

- Press a HotKey.

The label is added to the atom highlighted. If the label is a single element, such as "C", then the appropriate number of hydrogens are added to the label.

Figure 8-1 Labeling the α -atom using the HotKey "c"



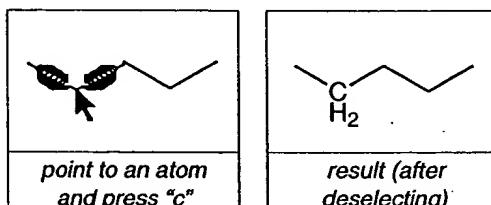
Method 3: Pointing at an atom using the Selection tool

- Using the Selection tool, position the pointer over an atom.

Highlight boxes appear over the bonds attached to the atom.

- Press a HotKey.

Figure 8-2 Labeling the β -atom using the HotKey "c"



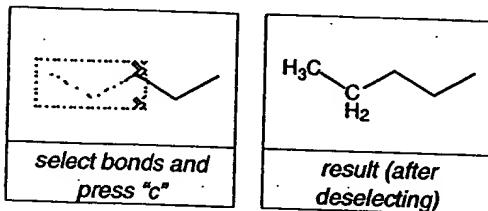
Method 4: Labeling atoms in a selection

- Select several atoms using the Selection tool.
- Press a HotKey.

The atoms whose bonds are completely selected are labeled.

The element or label associated with the HotKey is added to the structure. Only atoms with all their bonds selected are labeled. No label will result if all bonds to the atom are not selected.

Figure 8-3 Labeling several atoms using the HotKey "c"



Hard Coded HotKeys

Certain HotKeys provide other effects. These HotKeys are hard coded into ChemDraw and are not editable in the hotkeys.txt or ChemDraw HotKeys file. For instance, the HotKey "Enter" (or "Return") opens the atom label text box for the last atom drawn. See Table 8-1 for a list of hard coded HotKeys:

Table 8-1 Hardcoded HotKeys

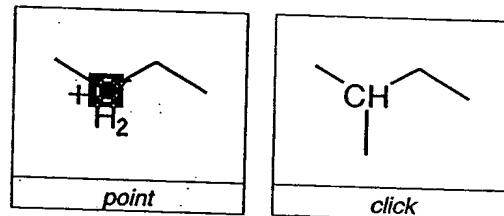
Press this HotKey	If you want to..
Enter (or Return) key	open the atom label text box.
space	remove an atom label.
/	display the Atom Properties dialog is opened. See "Atom Properties" in Chapter 9, Drawing Query Structures, for more information.
=	display the List Nickname dialog.
.	add an attachment point

Other HotKey Effects

Whenever new bonds are added to atoms that contain only a single element and hydrogen, the appropriate number of hydrogens will be added or removed from the label. This effect occurs for all labels regardless of their origin (HotKeys or the Text tool) if the atom label is set to Automatic justification. You can disable this effect if you choose Flush Left or another justification for the atom label.

For example, labeling an atom with CH₂ followed by adding a bond will result in a change to CH for the labeled atom. If you remove the bond, the label will return to CH₂.

Figure 8-4 Reducing the number of hydrogens when adding a bond



Creating HotKeys

To add or edit ChemDraw HotKeys::

Locate the file named "hotkeys.txt" in your cd_items directory or "ChemDraw HotKeys" in your ChemDraw Folder. Double-click its icon to open the file using Notepad, TeachText or the text editor of your choice. The file contains a simple list using the format shown in Figure 8-5. For example, the file in Figure 8-5 has the label COOH assigned to the "a" key, and the label CH3 assigned to the "c" key.

Any uppercase or lowercase alphanumeric key may be used as a HotKey with the exception of the hard coded HotKeys listed in Table 8-1. If a key is used more than once in the file, the one closer to the end of the file takes precedence.

Figure 8-5 Defining HotKeys in a text file

a COOH
b Br
c CH ₃
<i>HotKeys defined in text file</i>

To add a HotKey:

- Add a new line and type the key you want to use
- Type a space.
- Type the label to associate with the key.

Keep in mind, HotKeys defined for single elements will always result in the adding of the appropriate number of hydrogens.

If you are creating a new HotKeys file you should check for the following.

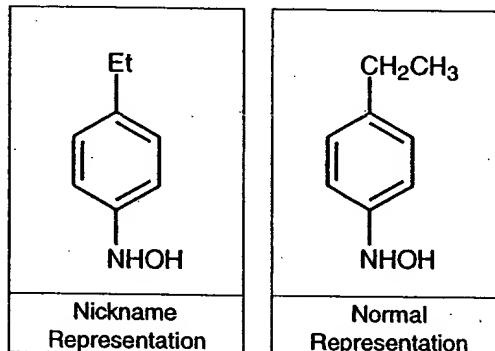
- Select a Text Only file format if you are using an application such as Microsoft Word.
- Type "hotkeys.txt" (Windows) (or "ChemDraw HotKeys" (Macintosh) for the file name.
- Select the cd_items directory (Windows) or the ChemDraw Folder (Macintosh) as the location to save the file.
- Click the OK (or Save) button.

NICKNAMES

Nicknames allow you to create shorthand representations for functional groups that you can use in as an atom label or as part of a label (the key here is that Nicknames are chemically meaningful whereas any random text is not).

Commonly used Nicknames, such as Me, Et, Ph etc. are provided with ChemDraw 3.5 in the nickname.dat or ChemDraw Nicknames file located in your cd_items directory (Windows) or ChemDraw Folder (Macintosh). However, you can easily add to this list, or delete those that you don't use.

Figure 8-6 Using a Nickname to represent an ethyl group



For added speed when using Nicknames, you can assign HotKeys to Nicknames. For example, in the Nicknames and HotKeys provided with ChemDraw 4.0, the HotKey, "4" labels an atom with "Ph" which is a Nickname representing a phenyl group. To learn more about HotKeys, see the previous section "ChemDraw HotKeys".

Using Nicknames

To use a Nickname to label an atom:

- Create a structure.
- Double-click an atom using a bond tool, or click an atom using the Text tool.

An atom label text box appears.

- Type a Nickname label such as "Et".

The atom is labeled with the Nickname, however, the chemical significance of the expanded structure is retained.

To select a Nickname to apply to an atom using a HotKey:

- Point to an atom.
- Press the HotKey “=”

The Nickname list appears.

- Select a Nickname from the list.
- Click the OK button.

To use a HotKey to label an atom with a Nickname:

- Using one of the labeling methods discussed in the earlier section, “Using HotKeys”, press a HotKey that defines a Nickname label. For instance press “4” to label an atom with “Ph”, or press “=” to open the List Nicknames dialog box where you can select a Nickname to use.

NOTE: Nicknames are tokens. As such, a Nickname will not flip orientation when applied to the left side of a structure when using Automatic Justification. For example, in the absence of a defined Nickname, the label “OTHP” will appear as “PHTO” when applied to the left side of a structure. However, since the Nickname “THP” is defined, the label appears as “THPO”. Also see “Automatic Justification” in Chapter 4, Captions and Atom Labels. To define your own Nicknames, you must have ChemDraw Pro.

PRO Defining Nicknames

To define a new Nickname

- Create a structure containing the functional group you want to define as a Nickname.
- Select the functional group.

There must be an atom that has some bonds selected and other bonds not selected indicating the connection point for the functional group. See the examples below.

NOTE: You can define Nicknames with either 1 or 2 connection points. However, the connection points must be single bonds.

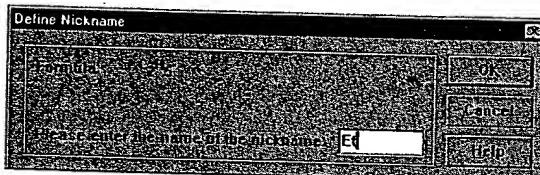
NOTE: If stereochemistry is indicated in a structure that you are defining as a Nickname, the stereochemistry is retained.

- From the Object menu, choose Define Nickname.

The number of connection points are shown by bullets after the Formula. You can have only one or two connection points in a nickname.

- Type a short name for the Nickname.
- Click the Define button.

Figure 8-7 Defining the Nickname “Et” for an ethyl group



The Nickname is defined, and you can now label atoms using its name.

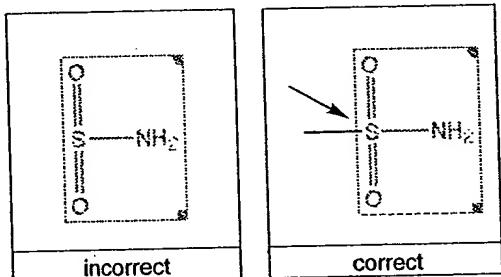
NOTE: If you use a name for your Nickname that is the same as an element name, you are alerted that the element will be replaced with the Nickname. For example using Ac for an acetyl group will replace the element Actinium. Further, the Check Structure and Analyze structure commands will recognize the label as an acetyl group rather than Actinium. Table 8-8 shows these conflicts. To return the proper interpretation of elements, choose List Nicknames from the file menu and delete the overriding Nickname definition.

Table 8-8 Default Nickname/Element name conflicts

Symbol	Nickname	Element
Ac	Acetyl	Actinium
Am	Amyl	Americium
Np	para-Nitrophenyl	Neptunium
Pr	Propyl	Praeseodymium

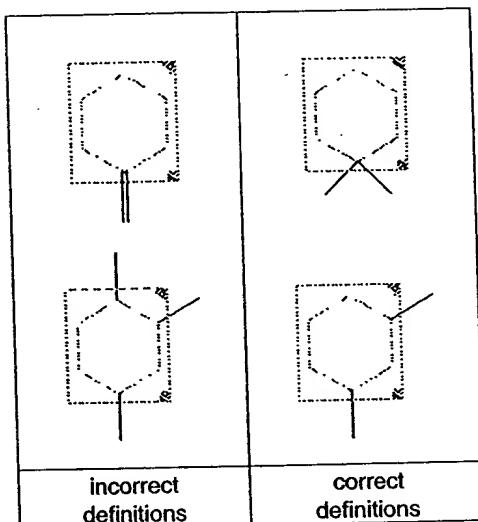
If, when defining a Nickname, the command Define Nicknames is dimmed, you have probably not allowed for a connection point or you have defined more than 2 connection points or the connection point is a double bond. In the example below, the functional group was drawn and the entire group selected. This is the incorrect way to define a Nickname since there is no atom that indicates a connection point. The Define Nicknames command is dimmed if you try to define a Nickname by this method. However, on the right, the sulfonamide group is attached to an unselected bond which defines a bond from sulfur as the connection point for the group. This is the correct way to define a Nickname.

Figure 8-8 Defining a Nickname with a single connection point



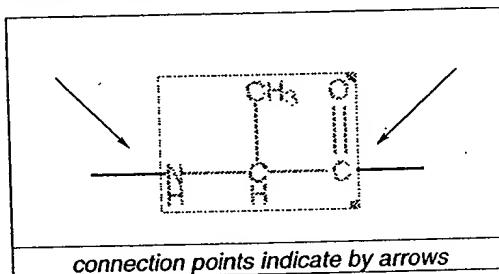
You must leave a bond unselected for each connection point. No more than two connection points can be defined in a nickname and no more than one attachment point on a single atom can be defined. Figure 8-10 shows some correct and incorrect definitions.

Figure 8-10 Defining Nicknames for groups that have two connection points



The definition in Figure 8-11 was used for the amino acid, Ala. The unselected bond at each end of the structure indicates the connection points; Nitrogen on the left and Carbon on the right.

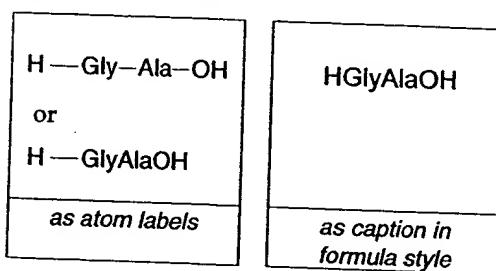
Figure 8-11 Further illustration of defining nicknames for groups with two connection points



connection points indicate by arrows

A peptide chain can be drawn by stringing these Nicknames together (Figure 8-12). Alternatively, you can string the Nicknames together in an atom label (below right), as long as there is a bond attached. Or, you can create a string of nicknames as a caption as long as formula style is applied.

Figure 8-12 Drawing a peptide chain by string together Nicknames



Viewing Nicknames

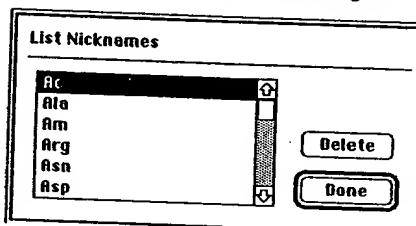
To view the list of defined Nicknames:

- From the File menu, choose List Nicknames.

The Nickname List dialog box appears.

Alternatively, you can use the "=" HotKey discussed in previous sections.

Figure 8-13 List Nicknames dialog box



Deleting Nicknames

To delete a Nickname.

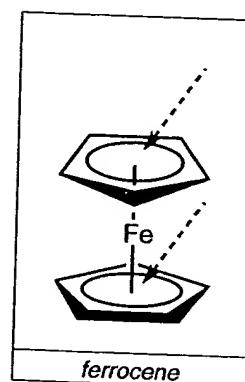
- Select the Nickname that you want to delete from the list.
- Click the Delete button.

The Nickname is permanently removed.

Multi-center Bonds

The multi-center attachment feature allows you to draw, with chemical significance, polyhapto structures, e.g. ferrocene ($(\text{Cp})_2\text{Fe}$). The basic procedure for drawing structures with multi-center attachments is to draw a fragment of the structure, select it, and designate it as a fragment with multi-center attachment. You can then attach bonds to that multi-center node created to represent the selected atoms.

Figure 8-14 Nodes defined for multicenter attachment



Creating a Multi-Center Bond

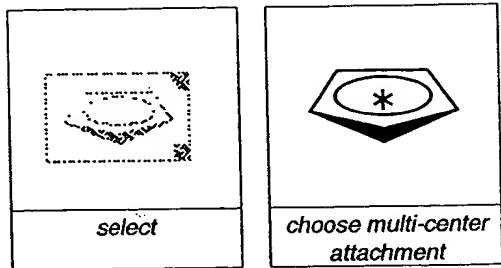
To create a multicenter attachment point:

- Select the structure whose center you want defined as a multi-center attachment point.
- From the Object menu, choose Add Multi-Center Attachment.

An asterisk is displayed with the fragment to show that it contains a multi-center node. This asterisk will not be visible once a bond is drawn to it.

NOTE: You can check that the multi-center attachment point is there by positioning the cursor over the attachment point using a structure drawing tool or the Selection tool. The asterisk will appear in the highlight box.

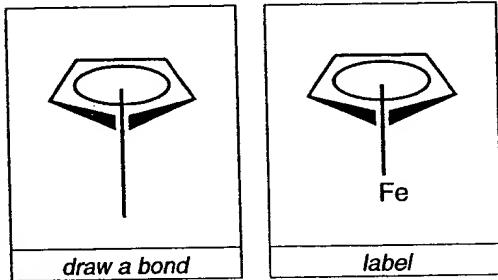
Figure 8-15 Creating a multicenter attachment point



To draw a bond to a multi-center attachment point:

- Select the Bond tool.
- Point to the asterisk and either click or drag to create a bond.

Figure 8-16 Drawing and labeling a bond from a multi-center attachment

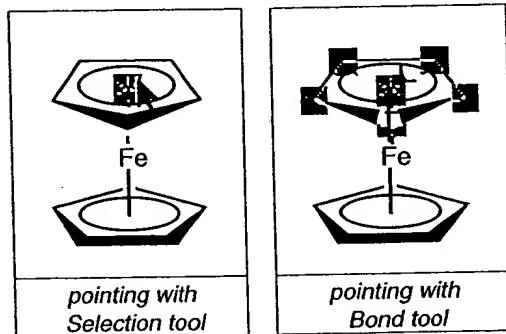


TIP: 1. To make the bond in ferrocene appear that it is coming from within the ring, double-click the wedged bond to make it come forward, or select the downward bond and choose Send to Back from the Object menu. 2. Double-click on the cyclopentadienyl ring with the Selection tool. Note that the entire structure, including the single bond, is selected. The Cp ring and the single bond are associated as one structural unit because the bond between them is recognized by ChemDraw.)

NOTE: For the best looking structure, you may want to toggle the Fixed Length command (by Command-L or Ctrl-L) to draw a longer than normal bond.

Once you draw a bond from the multi-center attachment point, the asterisk will disappear. However, you can check that the node is present by selecting a Bond tool or the Selection tool and positioning the cursor over the attachment point. If you use the Selection tool, only the attachment node will be highlighted. If you use the Bond tool, not only is the attachment node highlighted, but so are all of the atoms that it represents. This provides a way to check the definition of a pre-existing multi-center attachment point.

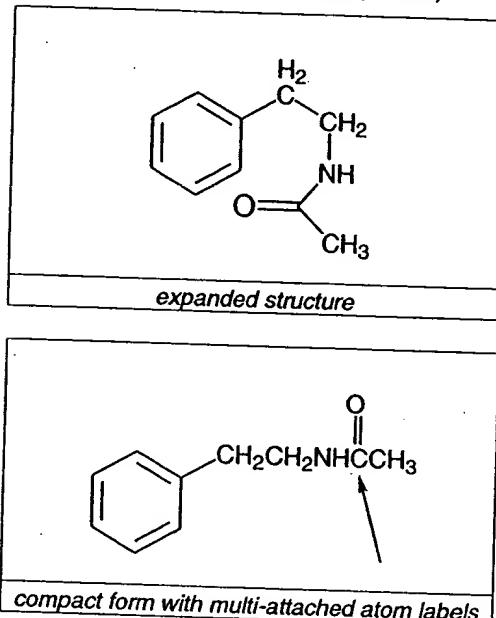
Figure 8-17 Pointing at an attachment point using different tools



Multi-attached labels

Multi-attached atom labels enable you to draw chemical structures more efficiently by allowing you to attach bond(s) anywhere along an atom label.

Figure 8-18 expanded (top) and compact form using multi-attached atom labels (bottom)



Adding Bonds to an Atom Label

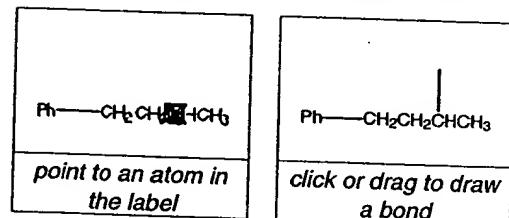
The basic procedure for drawing additional bonds to an atom labels is:

- Draw your structure and attach any necessary atom label.
- Select a Bond tool.
- Position the cursor over the part of the atom label to which you want to attach additional bonds. (The selected part of the atom label will highlight accordingly.)
- Click and drag from the atom label to draw your bond(s).

By dragging you can determine the orientation of the resulting bond. If you click to add a bond, there are several preferential orientations for the resulting bond as outlined below.

1. adding from the end of an atom label creates bonds that are preferentially horizontal.
2. adding from the middle of an atom label creates bonds that are preferentially vertical.
3. adding from the start of an atom label creates bonds that try to attain the chain angle setting in the Drawing Settings dialog box, otherwise the next best angle is used.

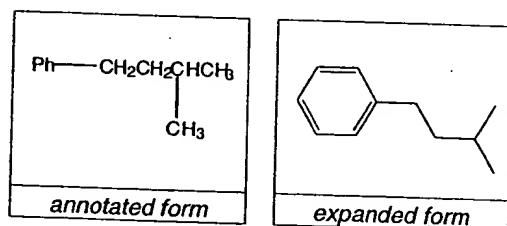
Figure 8-19 Adding a bond to an atom label



Expanding Labels

If you have drawn structures which contain defined nicknames or which contain long atom labels, you can have *ChemDraw* automatically redraw your structures in fully expanded form by choosing the Expand Label command from the Object menu.

Figure 8-20 Annotated and expanded form of a structure

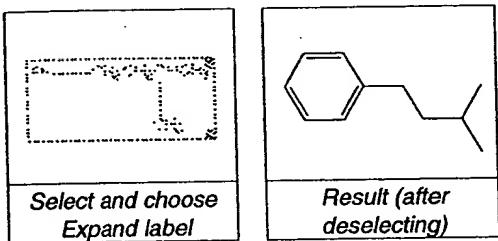


To expand atom labels:

- Select the Selection tool.
- Select the label within a structure that you want to expand, or double-click the structure to expand all possible labels.
- From the Object menu, choose Expand Label.

Your structure is redrawn in its expanded form.

Figure 8-21 Expanding all expandable labels in a selected structure



Structure Clean Up

The Clean Up Structure command, found in the Object menu is used to Neaten molecules by regularizing bond lengths and angles (graphic objects such as arrows and aromatic circles are not affected). You can use Structure Clean Up to redraw structures that you may have drawn freehand or to Neaten structures that you may have imported from another application.

Structure Clean Up will not necessarily create the best structure. Most structures have many "clean" forms, a problem that is particular noticeable with straight-chain alkanes.

If only part of a structure is selected when you choose Clean Up Structure, the other atoms and bonds will not be affected.

The salient points to note about structure clean up are:

- 1) The goal is to regularize bond lengths and bond angles to make for a more aesthetic picture.
- 2) Optimum bond lengths are determined by the Fixed Length in the Drawing Settings dialog.

3) A given ring is redrawn only if all of its constituent bonds are selected.

4) Clean is not good about complicated ring systems, particularly ones containing: trans double bonds; triple bonds; several highly connected rings; large rings.

5) Multi-attached atom labels and variable attachment points are not affected.

6) Multi-center bonds are not affected.

7) Structures are rotated so that as many bonds as possible are at a multiple of 15 degrees.

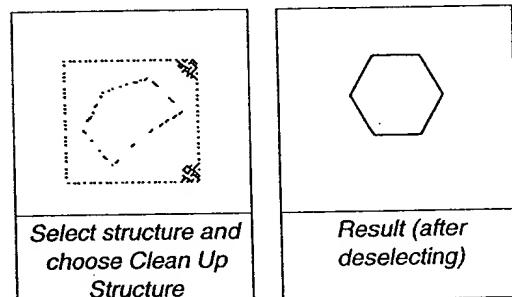
8) Structure cleanup will preserve stereochemical meaning rather than the precise identity of specific wedged and hashed bonds.

To use Structure Clean Up:

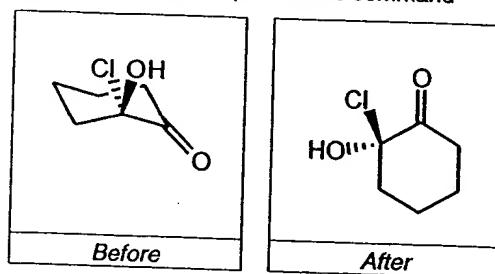
- Select the structure or part of the structure you want to clean up with the Selection tool.
- From the Object menu, choose Clean Up Structure.

NOTE: Clean Up Structure is not smart about positioning molecules relative to other objects. Overlap may occur.

Example 8-22 Applying the Clean Up Structure command



Example 8-23 Preservation of stereochemistry after applying the Clean Up Structure command



CHECKING CHEMISTRY

The Check Structure command and the Analyze Structure command provide ways to check your structure for valence and label errors, and calculate information about the structure.

NOTE: The Analyze command automatically performs the Check Structure command prior to the calculation.

Check Structure

You can check the chemistry of a selected structure, part of a structure or caption (in Formula style) using the Check Structure command. The algorithm for this command is based on normal valences and elements, and defined Nicknames.

To check the valences of all selected atoms in a structure:

- Select a structure, part of a structure, or caption using the Selection tool.
- From the Object menu, choose Check Structure

Each label in the structure is checked sequentially. When a label is incorrect, a message window appears. To continue checking the structure when a message appears:

- Click the Ignore button.

To ignore all subsequent errors in a structure:

- Click the Ignore All button.

To stop checking a structure when a message appears:

- Click the Stop button.

The atom that is causing the problem is selected.

Preferences Guide

Check Structure when Copying

To have ChemDraw perform a check structure analysis on any structure copied to the Clipboard:

- From the File menu, choose Preferences.
- Click the Check Structure When Copying checkbox.

This change affects all documents.

Figure 8-24 Message box indicating the error found during the Check Structure command

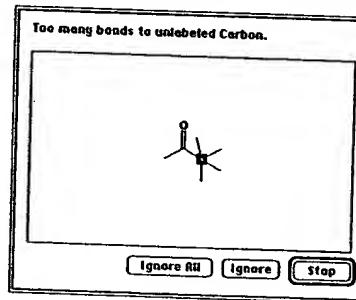
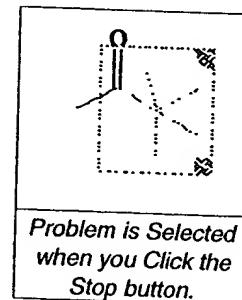


Figure 8-25 Error found during the Check Structure command



Analyze Structure

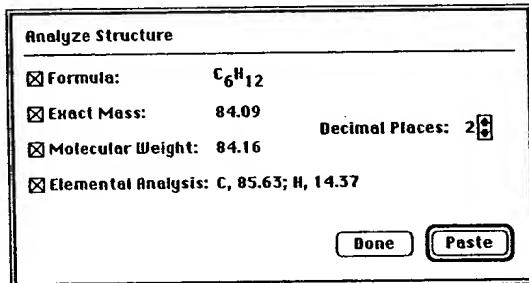
The Analyze command provides a quick way to generate the chemical formula, exact mass, molecular weight and elemental analysis for a selected structure, part of a structure or caption (in Formula style). Prior to the calculation, the Check Structure command is automatically performed.

To view information about a structure:

- Select an entire structure, part of a structure or a caption (in Formula style).
- From the Object menu, choose Analyze Structure

The Analyze Structure dialog appears. If any of the valences or labels are not correct you are alerted with a message. See "Check Structure" later in this document for more information. The example dialog box below shows information about a selected cyclohexane structure.

Figure 8-26 Analyze Structure dialog box for cyclohexane



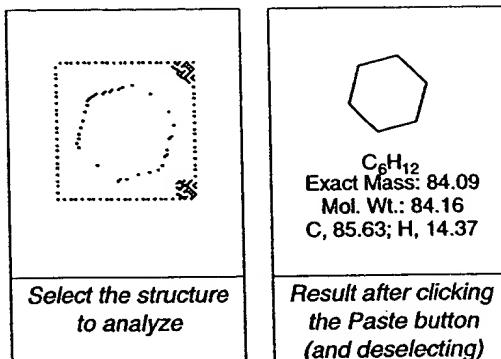
To paste information about a structure as a caption:

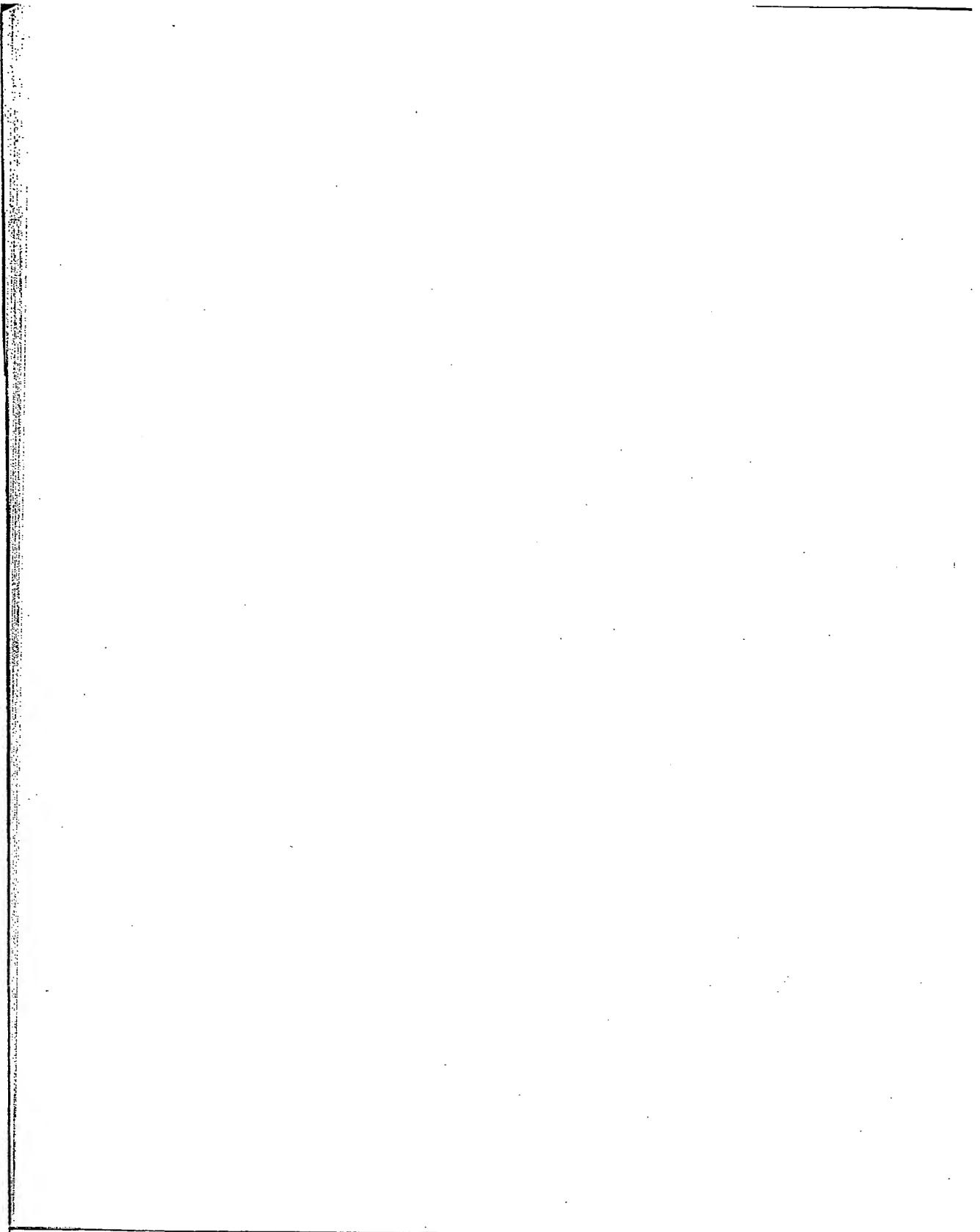
- Click the checkboxes for the information that you want to paste.
- Click the Paste button.

The information appears as a multi-line caption below the structure. This information can be edited using the text tool as you would any caption.

NOTE: Charge, radicals and isotopes are accounted for when using the analyze structure command. See Appendix A, The Chemistry of ChemDraw, for more information.

Figure 8-27 Analysis of cyclohexane





Chapter 9, Drawing Query Structures

WHAT ARE QUERY STRUCTURES?

Effective searching of chemical databases such as ChemFinder, DARC, or ISIS/Base is often most efficient when you specify properties for atoms and bonds in a query structure. Depending on the query structure you create, a more narrow or more broad search can be initiated. For instance, you might broaden a search by creating a query structure where you have applied bond properties indicating a bond as either double or single, or you might narrow a search by applying atom properties where a particular atom must have a charge of +3.

Because *ChemDraw* is not itself a chemical database application, the interpretation of query structures necessarily involves other programs. Not all databases support the same query properties. If you use a query structure containing properties not understood by a given database, you might get an error message from that database, or it might simply ignore the properties that it does not understand.

To use query structures for searching, you will likely be able to paste the query structure into a database's search window and initiate a search. Alternatively, you may need to save the structure in an appropriate file format and open the file in the database application.

A list of understood and not-understood properties for some database applications is provided in Table 9-13, later in this chapter. Also see "Transferring Information to Other Applications" in *Chapter 13, Sharing Information*, or consult the documentation for your chemical database.

NOTE: It is possible to assign conflicting or nonsensical properties. For example, you can require that one of the atoms in benzene is not part of any ring, which is inherently impossible. The resolution of this sort of impossibility depends on the query system used, but generally will result in no hits being found.

ATOM PROPERTIES

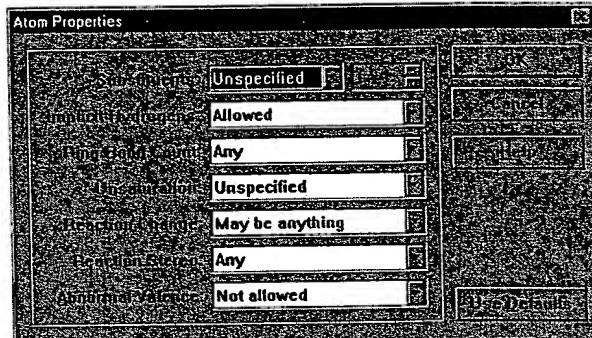
To assign properties to selected atom(s) in a structure:

- Select an atom by clicking with the Selection tool, or select multiple atoms by Shift+clicking.
- From the Object menu, choose Atom Properties or press the HotKey "/".

The Atom Properties dialog box appears.

- Select the atom properties from the drop-down list boxes that you want associated with the selected atom(s).

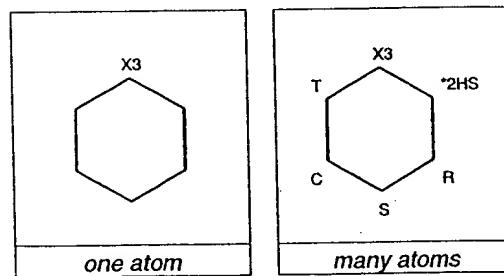
Figure 9-1 Atom Properties dialog box



- Click the OK button.

Small characters appear adjacent to atoms that have associated atom properties.

Figure 9-2 Atom properties associated with a single atom and many atoms



The character that appears depends on which query properties have been assigned. If more than one property is assigned, more than one character will appear adjacent to the atoms.

Table 9-1 Atom property indicators

Character	Query Property
*	Substituents: Free Sites (followed by the number of free sites)
U	Substituents: Up to (followed by the maximum number of substituents)
X	Substituents: Exactly (followed by the number of substituents)
H	Implicit Hydrogens
R	Ring Bond Count
S	Unsaturation
C	Reaction Change
T	Reaction Stereo

NOTE: The Abnormal Valence atom property does not provide any visual indicator. This allows you to use this property to disable Illegal Valence warnings for specific atoms without cluttering your structure diagram.

With the exception of the characters for the Substituents query property, the letters indicate only that a given property has been applied, and do not indicate the exact value of that property. To find the precise value of a query property setting:

- Select the atom.
- From the Object menu, choose Atom Properties.
- View the settings of the drop-down list boxes.

To remove atom properties from an atom:

- Select the atom.
- From the Object menu, choose Atom Properties.
- Click the Use Defaults button.

The atom properties are removed and the characters are no longer adjacent to the selected atom(s).

To remove specific atom properties:

- Select the atom.
- From the Object menu, choose Atom Properties.
- Select the default value for the atom property you want to (see the value labeled "default" in the Search Result descriptions below).

NOTE: You can view the atom properties for an atom using the HotKey "/". See "Using HotKeys to Label Atoms" in Chapter 8, Advanced Drawing Techniques.

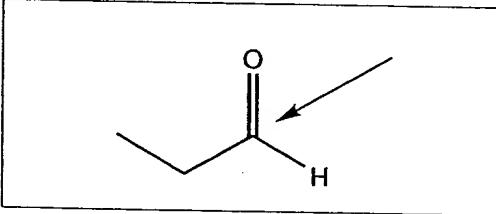
The following are the atom properties that you can associate with an atom:

Substituents

The Substituents property specifies the number of substituents bonded to the selected atom(s). In ChemDraw, a substituent is defined as a non-hydrogen atom connected by a bond of any order.

In Figure 9-3 below, the carbonyl carbon (indicated by the arrow) in propanal has a substituent count of two: the beta carbon and the aldehyde oxygen. This is because the double bond to the aldehyde oxygen counts as only one substituent (even though it is a double bond, it is still just one bond), and hydrogens never count as substituents.

Figure 9-3 The carbonyl carbon in propanal has a substituent count of two



The substituent count atom property allows you to specify the number of bonds to an atom in the target structure, including bonds already drawn in the query structure.

Table 9-2 Substituent options

Value	Search Result
Unspecified	<i>Default.</i> Behavior is determined by the target databases. Some databases (including ISIS) will find compounds with any substitution at this atom; some databases (including DARC) will find only compounds with substitution exactly as drawn.
Free Sites	Find compounds in which the selected atom(s) may contain a range of substituents up to the number specified in the spin control plus the number of bonds as drawn. A value of zero is equivalent to saying that the substituent count must be as drawn.
Up to	Find compounds in which the selected atom(s) may contain a range of substituents up to the number specified in the spin control.
Exactly	Finds compounds in which the selected atom(s) contains the exact number of substituents as specified in the spin control, up to 15 substituents.

Implicit Hydrogens

The Implicit Hydrogens property specifies whether additional, implicit hydrogens may be attached to the selected atom(s). If implicit hydrogens are disallowed, all valences to that atom must be filled by bonds to non-hydrogen atoms.

Table 9-3 Implicit Hydrogens options

Value	Search Result
Not allowed	Finds compounds with no additional hydrogens attached to the selected atom(s).
Allowed	<i>Default.</i> Finds compounds regardless of whether hydrogens are attached to the selected atom(s).

Ring Bond Count

The Ring Bond Count specifies the number of bonds attached to an atom that are part of rings of any size. For simple cases, this also implies the maximum number of rings in which an atom can reside.

Table 9-4 Ring Bond Count options

Value	Search Result
Any	<i>Default.</i> Finds compounds in which the selected atom(s) can be a member of any type of ring, or a member of no ring at all.
No ring bonds	Finds compounds in which the selected atom(s) is acyclic.
As drawn	Finds compounds in which the selected atom(s) resides in the same type and number of ring(s) as drawn.
Simple ring	Finds compounds in which the selected atom(s) is a member of only one ring (the atom has two ring bonds).

Table 9-4 Ring Bond Count options (*continued*)

Value	Search Result
Fusion	Finds compounds in which the selected atom(s) lies at ring fusions (the atom has three ring bonds).
Spiro or higher	Finds compounds in which the selected atom(s) is a member of a spiro or higher linkage (the atom has four or more ring bonds).

Unsaturation

The Unsaturation property specifies whether a multiple bond is attached to the selected atom(s).

Table 9-5 Unsaturation options

Value	Search Result
Unspecified	<i>Default.</i> Finds compounds regardless of whether a multiple bond is attached to the selected atom(s).
Must be absent	Finds compounds that do not have a multiple bond attached to the selected atom(s).
Must be present	Finds compounds that have a least one multiple bond (double, triple or aromatic) attached to the selected atom(s).

Reaction Change

The Reaction Change property specifies whether a change occurs at selected atom(s) after a reaction. This property is only meaningful when searching a database containing chemical reactions.

Table 9-6 Reaction Change options

Value	Search Result
May be anything	<i>Default.</i> Finds all compounds regardless of any change to selected atom(s) after a reaction.
Must be as specified	Finds all compounds that are changed at the selected atom(s) after a reaction as drawn.

Reaction Stereo

The Reaction Stereo property specifies that the selected atom(s) are stereocenters in a reaction. This property is only meaningful when searching a database containing chemical reactions.

Table 9-7 Reaction Stereo options

Value	Search Result
Any	<i>Default.</i> Finds all compounds regardless of the stereochemistry at the selected atom(s).
Inversion	Finds compounds whose the selected atom(s) has an inverted stereo configuration after a reaction.
Retention	Finds compounds whose selected atom(s) has an unchanged stereo configuration after a reaction.

Abnormal Valence

The Abnormal Valence property specifies whether selected atom(s) can have a valence other than normal. "Normal" valences for each element are defined in the Isotopes Table (Macintosh) or isotopes.txt file (Windows).

Table 9-8 Abnormal Valence Options

Value	Search Result
Not allowed	<i>Default.</i> Finds compounds where the selected atom(s) only has valences that are normal for that element. If necessary, hydrogen atoms are automatically added to or removed from the atom before transferring it to the chemical database. If the Check Structure When Copying to Clipboard or Exporting preference is turned on, an error message will warn of abnormal valences.
Allowed	Finds compounds with the specific valence drawn.

NOTE: If Abnormal Valence is Allowed, any Invalid Valence messages for those atoms will be ignored automatically by the Analyze Structure and Check Structure commands.

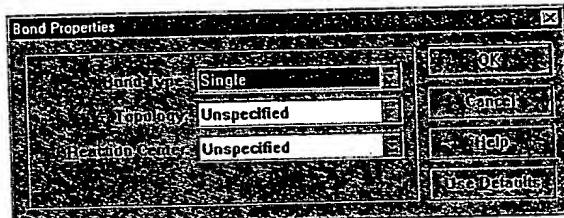
BOND PROPERTIES

To associate bond properties to selected bond(s) in a structure:

- Select a bond using the Selection tool, or Shift+click to select multiple bonds.
- From the Object menu, choose Bond Properties.

The Bond Properties dialog box appears.

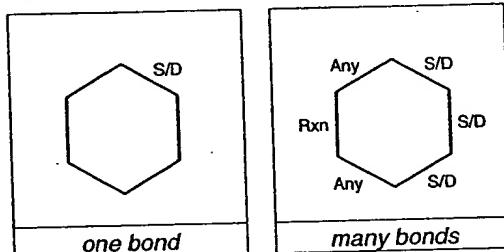
Figure 9-4 Bond Properties dialog box



- Select the bond properties you want from the various drop-down list boxes.
- Click the OK button.

Textual descriptors appear adjacent to bonds that have associated bond properties.

Figure 9-5 Bond properties associated with a single bond and many bonds



The descriptor that appears depends on which query properties have been assigned. If more than one property is assigned, more than one descriptor will appear adjacent to the atoms.

Table 9-9 Bond property indicators

Descriptor	Query Property
Any	Bond Type: Any
S/D	Bond Type: S/D
D/A	Bond Type: D/A
S/A	Bond Type: S/A
Rng	Topology: Ring
Chn	Topology: Chain
Rxn	Reaction Center

The descriptor for the Reaction Center query property indicates only that this property has been applied, and does not indicate the exact value of that property. To find the precise value of a query property setting:

- **Select the bond.**
- **From the Object menu, choose Bond Properties.**
- **View the settings of the drop-down list boxes.**

To remove all bond properties from selected bond(s):

- **Select the bond(s).**
- **From the Object menu, choose Bond Properties.**
- **Click the Use Defaults button.**

The bond properties are removed and the indicators are no longer adjacent to the selected bond(s).

To remove specific bond properties:

- **Select the bond.**
- **From the Object menu, choose Bond Properties.**
- **Select the default value for the bond property you want to remove (see the value labeled "default" in the Search Result descriptions below).**

The next sections describe the bond properties that you can associate with a bond(s).

Bond Type

This property specifies the bond type of the selected bond(s). The first portion of the pop-up menu changes the selected bond(s) to the type chosen. The remainder of the choices specify more complex query bond types.

The default bond type corresponds to the current type of the bond (single, double, etc.) as drawn.

Table 9-10 Bond Type options

Value	Search Result
Single..	Finds compounds with the bond type you select for the selected bond(s).
Dative	
Double or Double Bold	Finds compounds whose selected bond(s) is double.
Double Either	Finds compounds whose selected bond(s) is double bonds and have either <i>cis/trans</i> stereochemical configuration.
Aromatic	Finds compounds whose selected bond(s) is aromatic.
Tautomeric	Finds compounds whose selected bond(s) is tautomeric.
Triple	Finds compounds whose selected bond(s) is triple.
Any	Finds compounds regardless of the bond type of the selected bond(s).
S/D	Finds compounds whose selected bond(s) is single or double.
D/A	Finds compounds whose selected bond(s) is double or aromatic.
S/A	Finds compounds whose selected bond(s) is single or aromatic.

NOTE: Not all bond types are supported in all file formats. When an unsupported bond type is saved to a given file format, it is converted to the closest equivalent that is supported.

Topology

The Topology property specifies the ring environment of the selected bond(s).

Table 9-11 Topology options

Value	Search Result
Unspecified	<i>Default.</i> Finds compounds regardless of environment.
Ring	Finds compounds where the selected bond(s) is part of a ring.
Chain	Finds compounds where the selected bond(s) is part of a chain (and is specifically not part of a ring).

Reaction Center

The Reaction Center property specifies that the selected bond is affected in a reaction. This property is only meaningful when searching a database containing chemical reactions.

Table 9-12 Reaction Center options

Value	Search Result
Unspecified	<i>Default.</i> Finds compounds regardless of its being a reaction center.
Center	Finds compounds where the selected bond(s) is affected by a reaction, but the type of change is unspecified.
Make/Break	Finds compounds where the selected bond(s) is either broken or created in a reaction.

Value	Search Result
Change	Finds compounds where the bond order of the selected bond(s) changes in a reaction.
Make&Change	Finds compounds where the selected bond(s) is either formed or broken, and where its type changes in a reaction.
Not Center	Finds compounds where the selected bond(s) is not changed in a reaction.

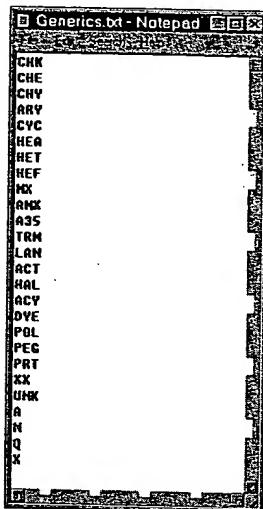
GENERIC NICKNAMES

Generic nicknames are nicknames that represent a class of elements or structural moieties. For example, "M" can be a generic nickname for all metals, "X" can represent halides, and "Ary" can represent an aromatic substructure. If you are using a query system that recognizes generic nicknames, you can use these nicknames in drawing your query in *ChemDraw*.

Generic nicknames, like other nicknames, can also be assigned HotKeys. For information on assigning a HotKey to a nickname, see "Creating HotKeys" in *Chapter 8, Advanced Drawing Techniques*. You cannot, however, define the meaning of a generic nickname within *ChemDraw* because generic nicknames represent multiple (and perhaps an infinite number of) substituents. Generic nicknames have meaning only in the context of the search system you are using.

The generic nicknames recognized as chemically meaningful by *ChemDraw* are listed in "Generic Nicknames" located in the *ChemDraw Folder* (Macintosh) or in "generics.txt" located in your *cd_items* directory (Windows). These files are text files similar to the HotKeys text files. To edit the generic nickname files, use a text editor such as Notepad to open the files, make your changes, and save your changes.

Figure 9-6 A sample Generic Nicknames text file

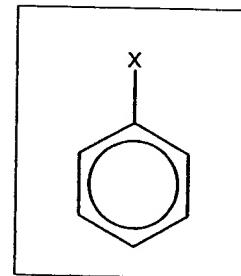


To label an atomic position with a generic nickname, use the same procedures as labeling an atom:

- Open a text box on an atom position by clicking with the Text tool, or double-click on an atom position with a Bond tool.
- Type the generic nickname you want.
- Press Return or click outside the text box.

NOTE: You cannot perform "Analyze Structure" or "Check Structure" on a structure with a generic nickname because, by definition, the structure contain variable substituents. If you do perform "Analyze Structure" or "Check Structure," the generic nicknames will be ignored and ChemDraw will report the chemical formula, mass, etc., as if the atom label containing the generic nickname were not selected.

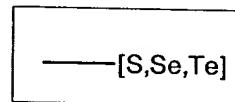
Figure 9-7 Using a generic nickname to specify X as any halogen.



ELEMENT LISTS

The element list allows you to define your search query more concisely. By labeling an atom position as a list of elements you specify that one of these elements must match in the structure for which you are searching. The elements in the element list must be separated by commas, but the brackets are optional. It is also optional to have a space after each comma.

Figure 9-8 An example of an element list



NOTE: An element list may contain only atomic elements, plus deuterium and tritium.

To create an element list:

- Open an atom label text box.
- Type an open bracket ("["), followed by a list of elements separated by commas ("Cl, Br, I"), followed by a close bracket ("]").

Figure 9-9 Creating an element list

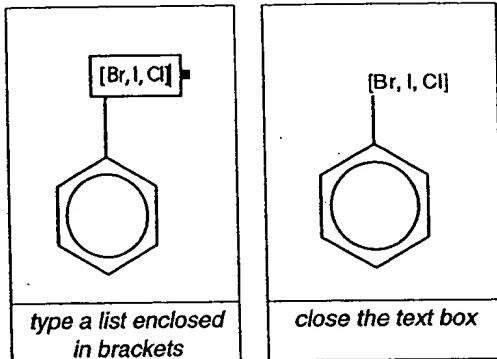
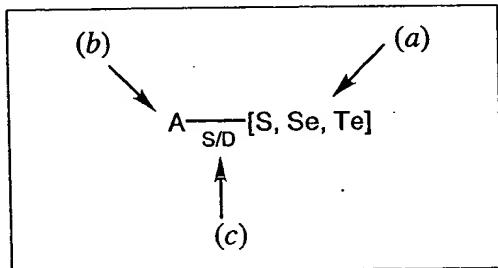


Figure 9-10 Creating a query structure to find compounds matching the following criteria:

- non-oxygen chalcogenide bonded to another atom;
- not necessarily carbon (a generic nickname);
- the bond type between the chalcogenide and the other atom to be a single or double bond.

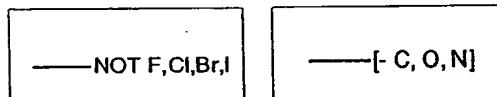


The "A" label denotes that the atom may match any atom except hydrogen. The mark near the bond indicates that the bond has special properties; in this case, in the Bond Properties dialog, you specified that the bond type must be single or double, S/D. Finally, by entering "S,Se,Te" enclosed in brackets, you specified that one of these elements must match in the target structures.

PRO ELEMENT NOT-LISTS

The element not-list is similar to an element list, but where an element list requires that one of the elements in the list matches the target structure, a not-list requires that the elements do *not* match. The elements in the element not-list must be separated by commas, but the brackets are optional. It is also optional to have a space after each comma. The word NOT must be in all-caps and must be followed by a space. Alternatively, the word NOT may be replaced with a minus sign.

Figure 9-11 Examples of element not-lists



NOTE: An element not-list may contain only atomic elements, plus deuterium and tritium.

To create an element not-list:

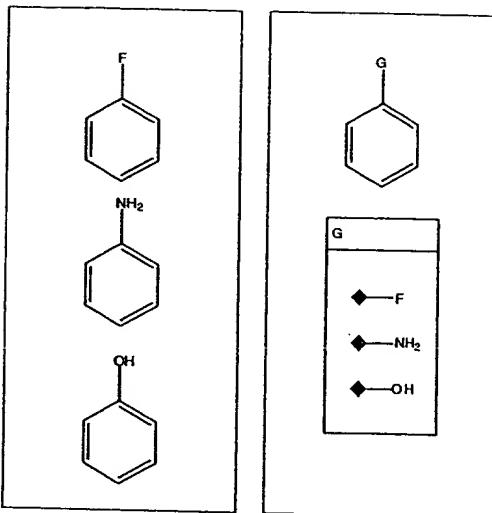
- Open an atom label text box.
- Type an open bracket, the word NOT, and a space ("[NOT ") followed by a list of elements separated by commas ("Cl, Br, I"), followed by a close bracket ("]").

PRO ALTERNATIVE GROUPS

The Alternative Group feature allows you to submit to your query system a search query that contains variable functional groups or substructures. Instead of submitting multiple queries on structures which share a common substructure, you can submit a single query with the parent structure. The parent structure would have attachment points to a list of alternative groups which you can define.

Alternative groups are also sometimes called R-Groups, S-Groups, G-Groups, or Generic Groups.

Figure 9-12 Defining an alternative group for the variable portion of the structure



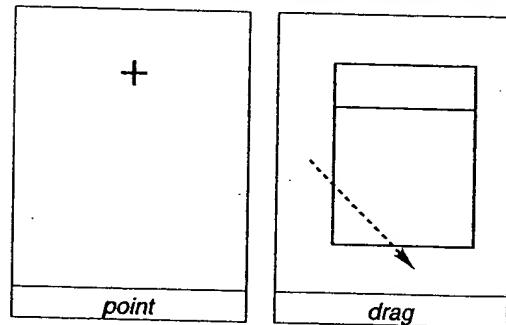
Defining an Alternative Group

Figure 9-13 Alternative Group tool



- Select the Alternative Group Tool.
- Click and drag in the *ChemDraw* window to create an area large enough for you to draw your alternative groups.

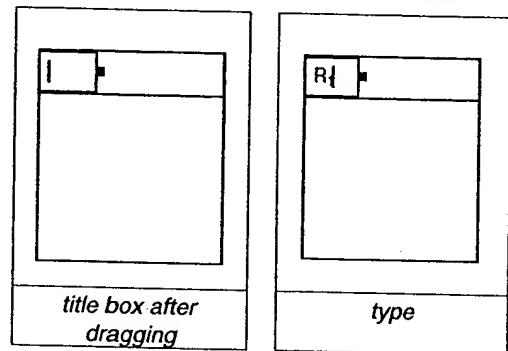
Figure 9-14 Creating an Alternative Group box



The Alternative Group Title box is automatically selected.

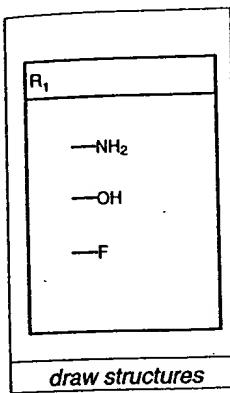
- Type a title, such as R₁, in the Alternative Group Title Box.

Figure 9-15 Creating an Alternative Group title



- Draw your substructure fragments in the Alternative Group Box.

Figure 9-16 Defining substructures



Next, you need to specify where your substructure fragments should be bonded to your parent structure at the Alternative Group Label. To label the attachment points, use the Attachment Point tool.

Figure 9-17 Attachment Point tool



- Select the Attachment Point Tool.
- Click on the substructure fragments where you want to place the attachment point. Or, you can use the HotKey ":".

An attachment point symbol appears where you click.

- Repeat for all fragments.

Figure 9-18 Assigning an attachment point to one fragment

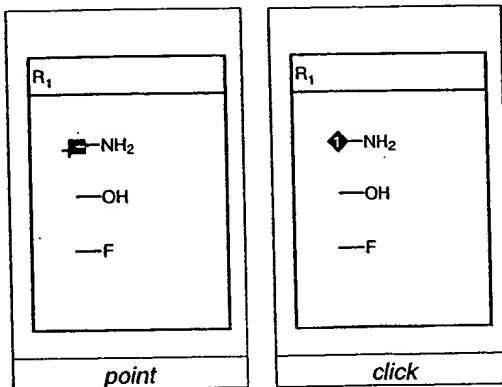
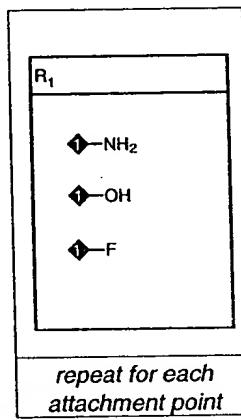
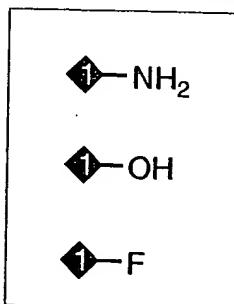


Figure 9-19 Alternative group fragments with attachment points



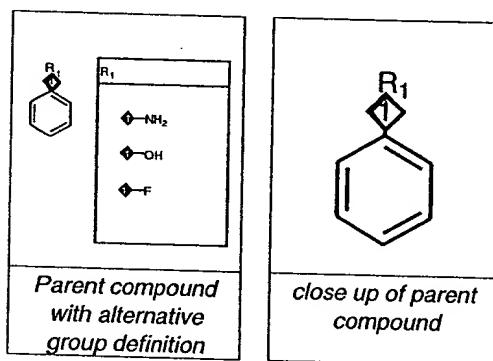
NOTE: The Attachment Points on your fragments are numbered. These numbers correspond to the Bond Rank number on your parent structure, and together they indicate how the structure fragments bond to the parent structure. For each fragment, the attachment point combined with the bond with the same bond rank number make up one bond.

Figure 9-20 Numbering of attachment points



When you create a parent compound containing the alternative group that you have defined, a attachment point symbol appears next to the label. The attachment point number matches those found in the definition.

Figure 9-21 Parent compound and alternative group definition



The numbering of the attachment points is related to the front to back order of the attachment points. To set the order of the attachment points, click the ends of the bonds in order. The last point clicked will have the highest number.

To change the ordering of the attachment points:

- Click the attachment points again with the Attachment Point tool.

- Or, select an attachment point with the Selection tool, and select Bring to Front or Send To Back in the Object menu.

The attachment point numbers are highest in the front.

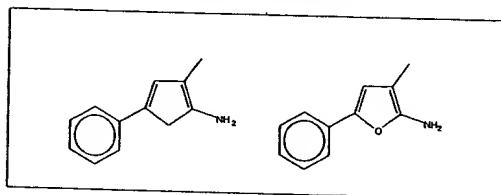
Having numbered attachment points is especially useful when you want to specify precisely how you want the structure fragments to be connected to your parent structure. For more information on structure fragments with multiple attachment points, see the following example.

NOTE: The completed query can be saved as an F1 Query file. The fragments that are not inside the Alternative Group Box will be interpreted as G0 in the F1 Query file. If the Alternative Group Labels are not G1, G2, G3, etc., they will be renamed when they are written out in the F1 Query format.

PRO MULTIPLE ATTACHMENT POINTS

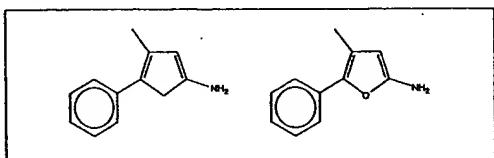
Having well-defined multiple attachment points on your structure fragments allows you to perform searches for specific materials. This type of search is especially useful if you are searching for conformationally similar structures. Suppose you want to find the two compounds below:

Figure 9-22 Targeted compounds



However, you are not interested in the two compounds below:

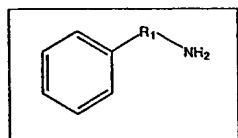
Figure 9-23 Undesired compounds



By specifying the attachment points order, you can exclude the unwanted hits. The parent structure below will satisfy the necessary requirements.

- Draw the parent structure shown below.

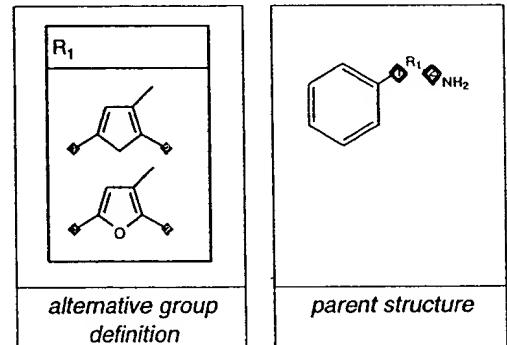
Figure 9-24 Parent Structure prototype



- Create an Alternative Group Box labeled "R1".
- Draw the structure fragments and label them with attachment points.

Once the alternative group definition is complete, the attachment point symbols will appear in the parent compound.

Figure 9-25 Complete alternative group definition and a parent



By clearly numbering your attachment points, you have unambiguously specified that the methyl group must be adjacent to the amine group. Thus, the conformers that you are not of interest are excluded.

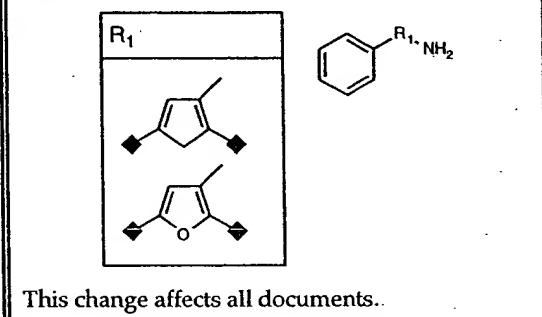
Preferences Guide

Show Attachment Rank Indicators

Sometimes — particularly in publication-quality drawings — the numbering of attachment points is implicit and the numbered attachment rank indicators are superfluous. To hide the attachment rank indicators and remove the numbers from the attachment points:

- From the File menu, choose Preferences.
- Deselect the Show Attachment Rank Indicators checkbox.

Figure 9-26 An alternative group definition and a parent structure with attachment rank indicators hidden.



This change affects all documents.

PRO ANONYMOUS ALTERNATIVE GROUPS

An anonymous alternative group is a cross between an element list and an alternative group. Where element lists are restricted to single elements only, anonymous alternative groups can contain any structure that can be represented in a textual form. Nicknames and generic nicknames are allowed in anonymous alternative groups. Anonymous alternative groups are a "shortcut" notation for regular alternative groups, eliminating the need to specify a name such as "R1" (hence, anonymous).

As with element lists, the anonymous alternative group allows you to define your search query more concisely. By labeling an atom position as a list of substructures you specify that one of these substructures must match in the structure for which you are searching. The items in the anonymous alternative group must be separated by commas, but the brackets are optional. It is also optional to have a space after each comma.

Figure 9-27 Some examples of anonymous alternative groups

— [OMe,OPh]	— [M,B,C]
— [OCH ₃ ,OH]	— X,S,Se

The procedure for creating anonymous alternative groups is similar to creating element lists:

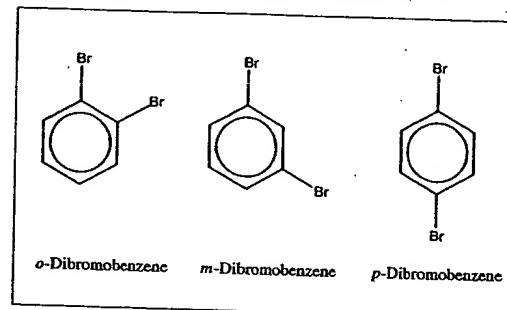
- Open an atom label text box.
- Type an open bracket ("[") followed by a list of elements, fragments, nicknames, or generic nicknames separated by commas, followed by a close bracket ("]").

VARIABLE ATTACHMENT POSITIONS

The Add Variable Attachment command, found in the Object menu, allows you to draw different positional isomers of a compound using an abbreviated notation that retains chemical significance.

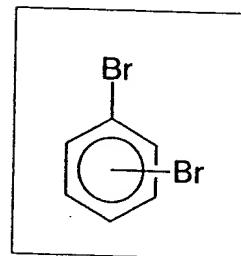
For example, you can draw explicitly the three isomers of dibromobenzene shown in Figure 9-28.

Figure 9-28 Explicit isomers of dibromobenzene



Or, through the use of variable attachment, you can express all three isomers as a single parent structure as shown in Figure 9-29.

Figure 9-29 Parent structure for representing isomers of dibromobenzene



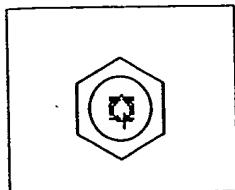
The procedure for using variable attachment is similar to adding multi-center attachment.

- Draw the structural fragment to which you want to assign a variable attachment node.
- Select the fragment using the Selection tool.

- From the Object menu, choose Add Variable Attachment.

An asterisk with a dot appears in the center of your fragment (Figure 9-30).

Figure 9-30 Structure with a variable attachment point

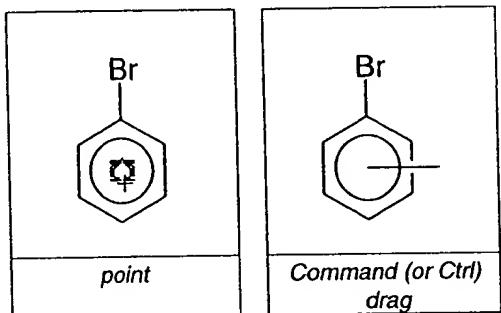


You can treat this attachment node just as you would treat the end of a normal bond.

- Select a Bond tool.
- Drag to draw bond.

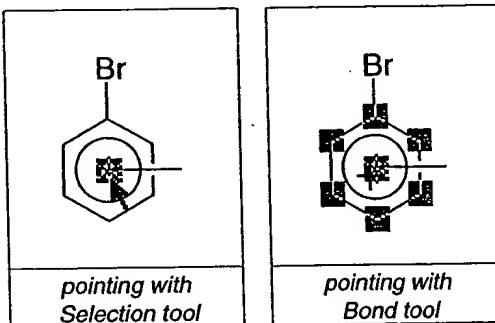
NOTE: In the example below (Figure 9-31), fixed lengths was disabled (using the Command key (Macintosh) or Ctrl key (Windows), so a bond could be drawn extending further from the ring.

Figure 9-31 Drawing a bond from a variable attachment point node



Once you draw a bond from the attachment node, the asterisk will disappear. However, you can check that the node is present by selecting a Bond tool or the Selection tool and positioning the cursor over the attachment point. If you use the Selection tool, only the attachment node will be highlighted. If you use the Bond tool, not only is the attachment node highlighted, but so are all of the atoms that it represents. This provides a way to check the definition of a pre-existing attachment node.

Figure 9-32 Pointing to a variable attachment point node



PRO EXPORT COMPATIBILITY

Since query properties are only useful in the context of a chemical database, it is necessary to transfer your structures from *ChemDraw* into your search system. Unfortunately, not all file formats support the same query properties, and not all chemical databases support the same file formats. Consult the documentation for your database to see which file formats it supports.

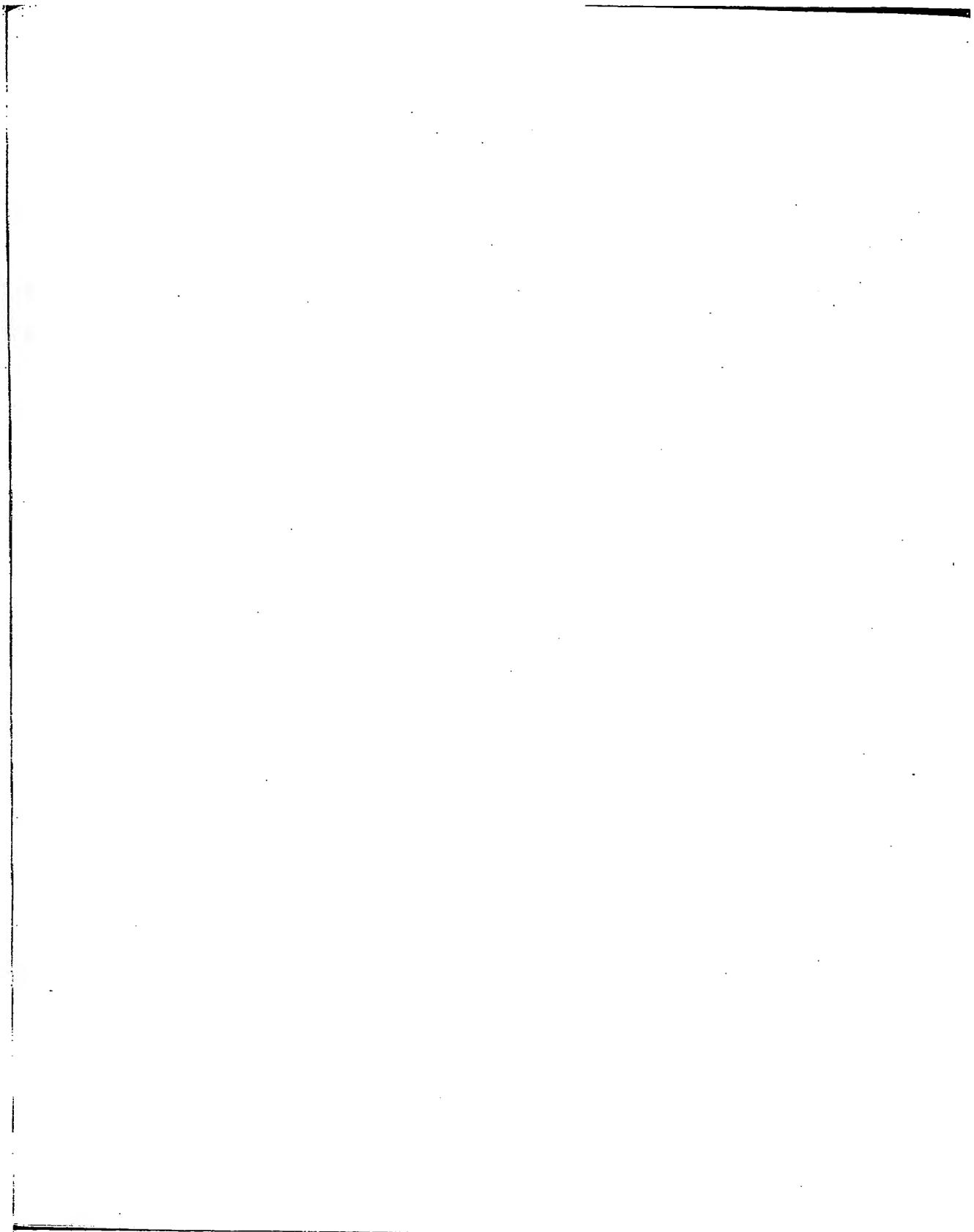
Table 9-13 is a list of the query properties that *ChemDraw* writes to ISIS (SKC, TGF, and Clipboard) and DARC (F1, F1-Query, and Clipboard) file formats. All query properties are written to the *ChemDraw* 4.0 (CDX) file format. CDX is the preferred format to use when you want to retain all query properties in a drawing, but might not be compatible with your database system.

Table 9-13 Exported query properties

	ISIS	DARC F1-Query	ISIS	DARC F1-Query
ATOM PROPERTIES				
Substituents				
Unspecified	✓	✓		
Free Sites		✓		
Up to		b		
Exactly	✓			
Implicit Hydrogens				
Not allowed	✓			
Allowed	✓			
Ring Bond Count				
Any	✓			
No ring bonds	✓			
As drawn	✓			
Simple ring	✓			
Fusion	✓			
Spiro or higher	✓			
Unsaturation				
Unspecified	✓			
Must be absent	✓			
Must be present	✓			
Reaction Change				
May be anything	✓			
Must be as specified	✓			
Reaction Stereo				
Any	✓			
Inversion	✓			
Retention	✓			
Abnormal Valence				
Not Allowed	✓	✓		
Allowed	✓	✓		
BOND PROPERTIES				
Bond Type				
Single			✓	✓
Dashed			✓	d
Hashed			d	d
Wedge Hashed			✓	✓
Bold			✓	e
Wedge			✓	✓
Wavy			✓	f
Hollow Wedged			d	e
Dative			g	g
Double			✓ ^b	✓
Double Either			✓	✓
Double Bold			i	i
Aromatic			✓	✓ ⁱ
Tautomeric			k	k
Triple			✓	✓
Any			✓	✓
S/D			✓	✓
D/A			✓	✓
S/A			✓	✓
Topology				
Unspecified			✓	✓
Ring			✓	✓
Chain			✓	✓
Reaction Center				
Unspecified			✓	
Center			✓	
Make/Break			✓	
Change			✓	
Make&Change			✓	
Not Center			✓	

Table 9-13 Exported query properties (continued)

	DARC	
	ISIS	F1-Query
OTHER QUERY ATTRIBUTES		
Generic Nicknames	^m ✓	✓ ^a
Element Lists	✓ ^b	✓
Element Not-Lists	✓ ^c	
Alternative Groups	✓ ^d	
Anonymous Alternative Groups		
Variable Attachment Positions		
^a Free Sites counts of zero translated to "Substitution as drawn"; all other Free Sites values unsupported		
^b Converted to the appropriated number of Free Sites		
^c Substituent counts of greater than 5 are translated to "6 or more"		
^d Converted to Wedged Hashed		
^e Converted to Wedged		
^f Converted to Racemic		
^g Converted to a Single, with a positive charge applied to that atom at the base of the dative bond and a negative charge applied to the atom at the point of the dative bond		
^h Interpreted by ISIS as unspecified <i>cis/trans</i> stereochemistry		
ⁱ Converted to Double		
^j Converted to Normalized		
^k Converted to S/D		
^l Converted to Undefined		
^m Only M, X, Q, A		
ⁿ Extensive list — see DARC manual		
^o Truncated to the first 5 elements		
^p Converted to G-Groups and possibly renamed; only 20 supported in one file		



Chapter 10, Drawing With Templates

Template documents are collections of structures organized by structural type or functionality. A structure in a Template document is named a template. You can use an existing template instead of drawing the structure to shorten the time required to create documents.

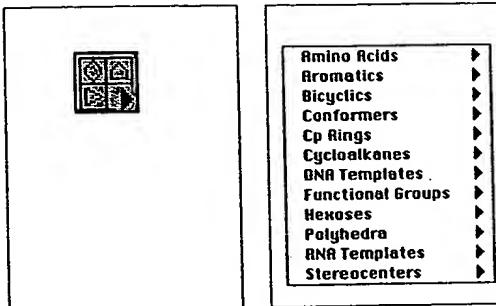
The Template documents distributed with *ChemDraw* are stored in a directory named "cd_items" (Windows), or in a folder named "ChemDraw Folder" (Macintosh) that usually resides in the same folder/directory as the *ChemDraw* application.

PRO In *ChemDraw Pro* you can define your own commonly used structures as templates. Any Template documents in the *ChemDraw* Folder are listed in the Windows menu in *ChemDraw Pro*.

THE TEMPLATE TOOL

Several tools, including the Template tool, contain palettes from which you can select many different types of structures or objects. The triangle in the lower right corner of the picture of the Template tool indicates that this tool contains a palette. The Template tool has two levels: the first level displays the available Template documents, and the second level displays the templates within each Template document.

Figure 10-1 Template tool icon and file list



To display the available Template documents:

- Point at the Template Tool icon in the Tools palette and hold down the mouse button.

A menu listing the Template documents appears. Template documents must be stored in the cd_items directory (Windows) or in the ChemDraw Folder (Macintosh) to appear in this menu.

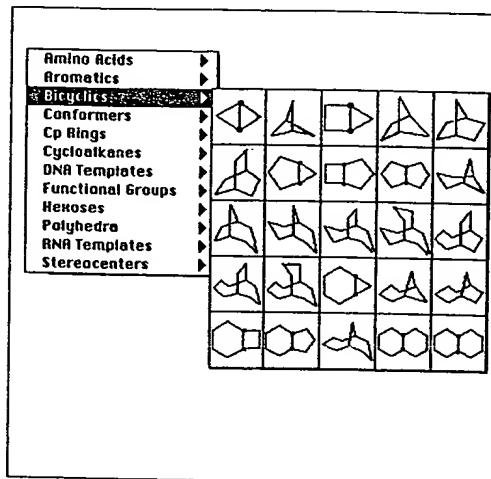
NOTE: **PRO** In *ChemDraw Pro* the pop-up menu is segmented if any Template documents are open for editing. The upper segment contains Template documents that are currently open for editing.

To display the templates available within a particular Template document:

- Drag to the name of the Template document and continue holding the mouse button down.

A palette appears containing the available templates.

Figure 10-2 Bicyclics template displayed using the Template tool



Choosing a Template

To choose a template from a Template palette:

- Point to the Template Tool icon and hold down the mouse button.
- Drag to a Template document name and then to a template.
- Release the mouse button to choose the highlighted template.

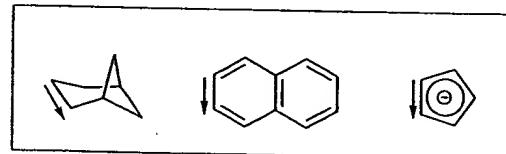
NOTE: **PRO** In ChemDraw Pro (Macintosh only) when you choose a template, the template document containing the template is added to the Window menu. Choosing the document from the Window menu opens it for editing.

NOTE: When you display the Template palette that was last used, a blinking box appears around the currently selected template until you drag to another template.

DRAWING WITH TEMPLATES

Drawing with templates is similar to drawing with the Ring Tools discussed in *Chapter 3, Drawing Chemical Structures*. When you draw with templates, the first bond drawn determines the position of the template in a document window and all remaining bonds are drawn counterclockwise. The most nearly vertical bond on the leftmost atom is drawn first, from top to bottom. If there are two equivalent bonds, the atoms that are at a lower position are used to draw the first bond.

Figure 10-3 Drawing direction of template structures



Templates are automatically scaled to the document settings of the current document in the active window (see "Autoscaling" in *Chapter 13, Sharing Information*). Once a template is drawn in a document window, the structures or objects can be manipulated by standard drawing and editing methods.

To quickly draw a template:

- Click in a document window.

The template is drawn centered around the pointer in the orientation that it appears in the Templates palette.

To quickly draw a template and fuse it with an existing structure:

- Click an existing bond in a document window.

To deposit a template and create a spiro-linkage with an existing structure:

- Click an existing atom in a document window.

To draw a template in a document window and control the size and orientation:

- Drag from the beginning of the first bond in the template to the end of the first bond.

When you drag upwards the bulk of the template is drawn to the left, and when you drag downwards the bulk of the template is drawn to the right. Templates must contain at least one bond in order to be drawn by the dragging method.

Drawing with the Same Template

To draw another template of the same type:

- Click the **Template Tool icon** to select it.
- Draw the template in a document window.

PRO CREATING TEMPLATES AND TEMPLATE DOCUMENTS

In *ChemDraw Pro* you can create new templates and add them to existing Template documents or create new Template documents.

To create a new Template document (Windows):

- From the **File menu**, choose **Open Special**.
- From the **Open Special submenu**, choose **TEMPLATE.CTS**.

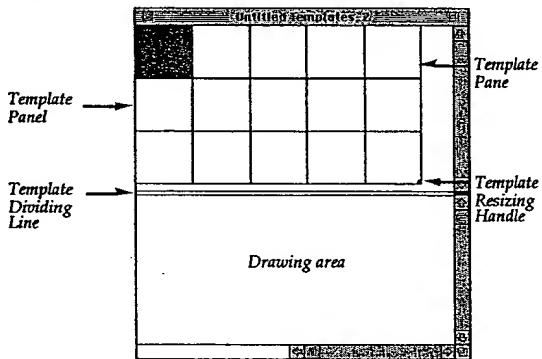
Or, for the Macintosh:

- From the **Window menu**, the **New Template stationery pad**.

A new and untitled Template window appears. The Template window is similar to a document window regarding the standard window elements, such as scroll bars. In addition, the Template window is divided into two halves by a moveable, horizontal line. The top half of the window is the Template panel that consists of individual Template panes where newly created templates will appear. The bottom half of the window is the drawing area where you can draw new templates.

NOTE: The templates you define are not limited to atoms and bonds. Templates can contain any ChemDraw object such as captions, boxes, arcs, orbitals, arrows, reaction mechanism symbols and curves. The ChemDraw objects in Template documents can also be colored. However, the colors will not appear in the Template tool pop-up palette. You can also paste pictures from other applications into a Template pane. Pasted objects are scaled to the current Template document settings, (see "Autoscaling", Chapter 13, *Sharing Information*, for more details). Templates must contain at least one bond in order to use the dragging method to draw in a document window.

Figure 10-4 A Template window



Creating Templates

To create a new template:

- Select a **Template pane** by clicking it.
- Draw a **structure or object** in the **drawing area** of the **Template window**.

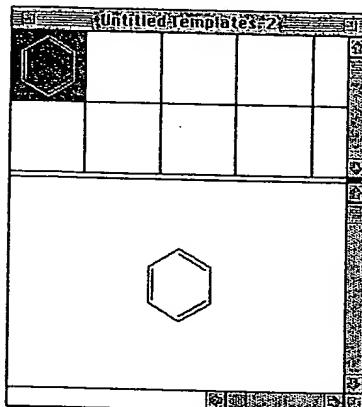
The structure appears in the Template pane as you draw. The tools in the Tools palette are used to draw a template in the drawing area of the Template window exactly as they are used to draw structures in the drawing area of a document window.

To select a different Template pane:

- Click another Template pane.

When you select a Template pane, the contents of the pane appear in the drawing area.

Figure 10-5 Creating a template



As you define templates they become available for use in your document without having to save the Template document.

- Point at the Template Tool icon in the Tools palette and hold down the mouse button.

The name of the new Template document appears in the pop-up menu.

Orientation of Templates

To make the templates that you create as easy to draw with as possible, it is recommended that you orient your structures so that the bond that establishes the position of the template, for instance the bond used for fusing, is leftmost and vertical. As discussed in "Drawing a Template" earlier in this chapter, the most vertical leftmost bond is drawn first. Refer to that section for examples.

Resizing Template Panes

To resize the Template panes in the Template panel:

- Drag the Resize handle on the lower right corner of the Template panel.

The percentage the block of Template panes is enlarged or reduced appears in the Message area.

Template Panels

To increase the size of the Template panel:

- Drag the Template dividing line.

To add a row of panes to the Template panel:

- Select a Template pane.
- From the Tools menu, choose Add Row.

The new row is added at the below the Template pane you selected.

To add a column to the Template panel:

- Select a Template pane.
- From the Tools menu, choose Add Column.

The new column is added to the right of the Template pane you selected.

To delete a row of Template panes from the Template panel:

- Select a Template pane in the Row you want to delete and choose Delete Row from the Tools menu.

To delete a column of Template panes from the Template panel:

- Select a Template pane in the column you want to delete.
- From the Tools menu, choose Delete Column.

The column is removed and all other columns are moved to the left.

Saving Template Documents

To save a Template document and have it available in the Template pop-up menu and the Window menu:

- From the File menu, choose Save As.

The Save File dialog box appears (Figure 10-6). The *cd_items* directory (Windows) or the *templates file format* are automatically selected.

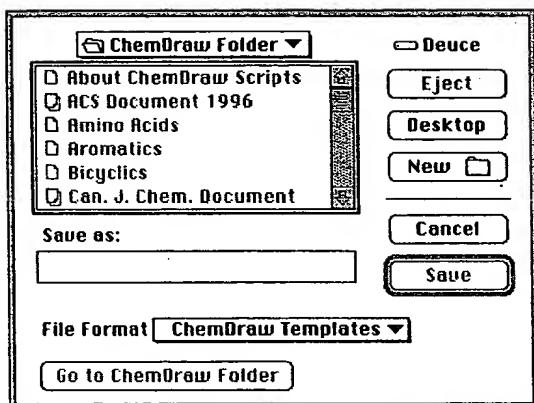
Windows: Saving a Template document in the *cd_items* directory makes it accessible in the Open Special submenu and in the Template tools palette.

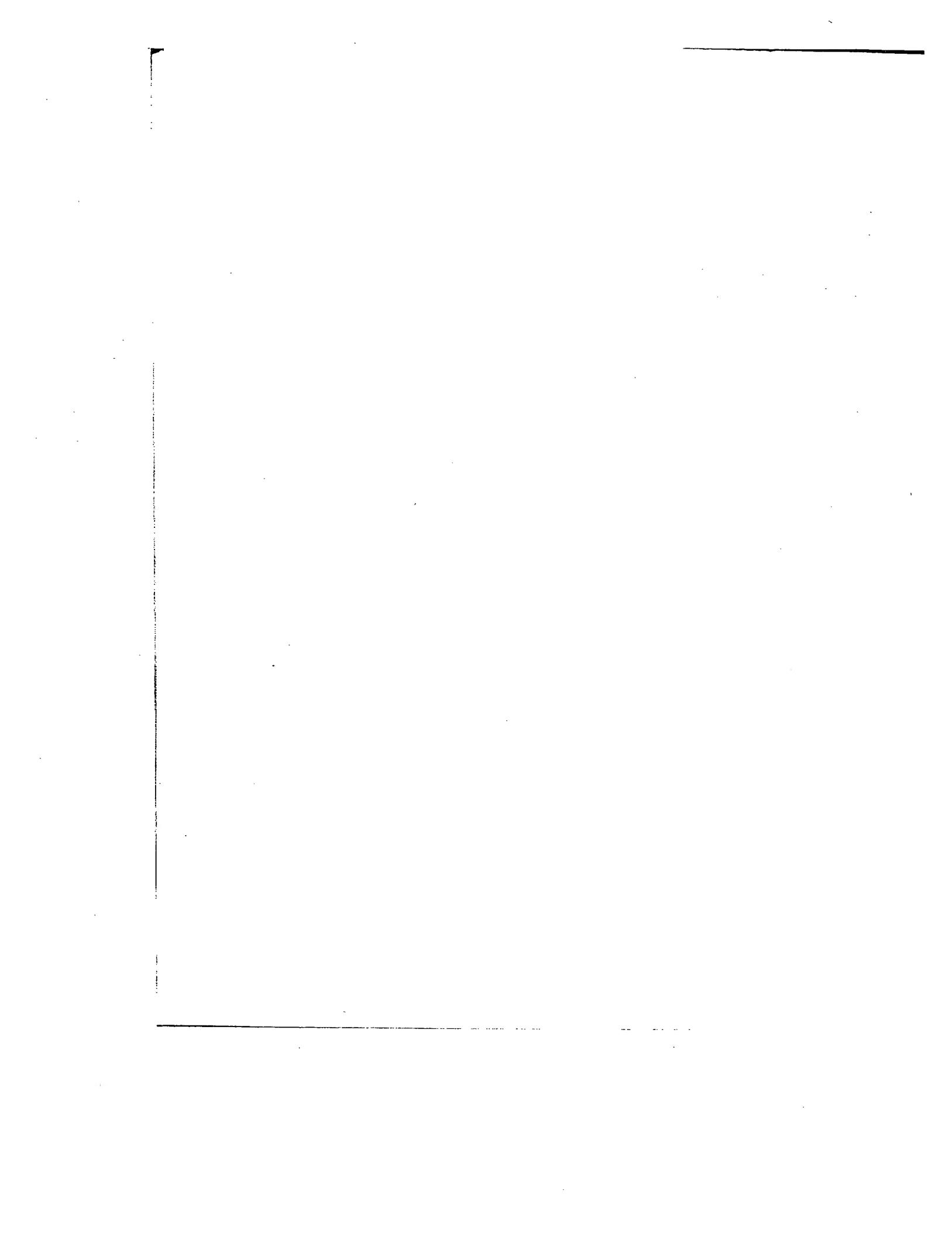
Macintosh: Saving a document in the *ChemDraw* Folder makes it accessible in the Windows menu and in the Template tools palette.

- Type a name for the Template document and click the OK/Save button.

The Template document will be available for use each time you start *ChemDraw Pro*.

Figure 10-6 The Save dialog box (Macintosh) when saving a template





Chapter 11, Working with Color

With the color capabilities of *ChemDraw*, you can create full color presentations of your chemical drawings to appear on your monitor, print on a color printer, or create 35mm slides using a film printer.

Most computers can display any of 16 million colors, but the number of colors that can appear at any one time may be limited by the particular monitor and display card installed in your computer.

In *ChemDraw* you can choose from a palette consisting of a Background Color, a Foreground Color, and up to twenty additional colors for any given drawing. A palette is stored in every document and style sheet/stationery pad. You can use style sheets/stationery pads to create a series of documents with the same color scheme. For more information on style sheets/stationery pads, see "Saving Customized Settings" in *Chapter 1, ChemDraw Basics*.

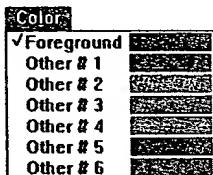
Using color you can:

- Color atoms and bonds in a mostly black-on-white drawing to highlight areas of interest.
- Color parts of a structure in a reaction scheme to indicate where starting materials end up in the products of a complicated mechanism.
- Use colored boxes and circles to highlight atoms or molecules.
- Create slides that are easier to view by using light objects on a dark background.

COLOR MENU

The Color menu contains the palette of colors that you can use to color objects and text in the document within the active window.

Figure 11-1 The Color menu



The Foreground color in the Color menu is the color used for all newly drawn objects. The Other colors in the Color menu can be used to change the color of objects that you select.

You can customize the Color menu using the Color Palette dialog box in the File menu. Colors can be added, or existing colors can be changed. Changing a color, for instance Other #2, changes all objects that are using the color.

NOTE: If you select an individual or grouped object that contains multiple colors, there will be a check mark next to each of the colors in the Color menu. The purpose of the check marks is to alert you that a change would affect more than one color.

Coloring Objects

Any object that you can select with the Selection tool can also be colored.

To color an object:

- Select the object in a document window using the Selection tool.
- From the Color menu, choose a color.

You can color individual bonds, part or all of a chemical structure, or objects such as boxes, curves, arrows, orbitals and reaction mechanism symbols.

The border of objects that are shaded or filled, such as white filled s-orbitals in the Orbitals palette, will be the same color as the shading or fill. The border of objects that are hollow, such as circles and hollow boxes in the Drawing Elements palette can be colored, but the inside of the object cannot.

Coloring Text

This section discusses coloring caption and atom label text.

Captions

Captions can be colored before or after they are typed, and can be colored as a whole or in part.

To color a caption:

- Select the Text tool.
- Click in the position where you want to place the caption.
- From the Color menu, choose a color.
- Type a caption.
- Press Enter to close the Caption text box.

NOTE: Which key you use to close the Text box will depend on the current setting for the "Require Option+Return (or Ctrl+Enter) to Create New Line preference in the Preferences dialog box.

To color individual characters:

- Select part of an existing caption using the Text tool.
- From the Color menu, choose a color.

NOTE: Captions that contain multiple colors will change to the foreground color when rotated. However, all colors contained in the caption are printed.

To color several captions at once:

- Select the captions using the Selection tool.
- From the Color menu, choose a color.

Atom Labels

You can change the color of an atom label either before or after you type it.

To color an atom label before it has been typed:

- Click an atom using the Text tool.
- From the Color menu, choose a color.
- Type an atom label.
- Press Enter.

NOTE: Which key you use to close the Text box will depend on the current setting for the "Require Option+Return (or Ctrl+Enter) to Create New Line preference in the Preferences dialog box.

- Select part of an existing atom label using the Text tool.

- From the Color menu, choose a color.

To color several atom labels at once:

- Select the atom labels using the Selection tool.
- From the Color menu, choose a color.

NOTE: Atom Labels that contain multiple colors will change to the foreground color when rotated. However, all colors contained in the atom label are printed.

CHANGING THE COLOR PALETTE

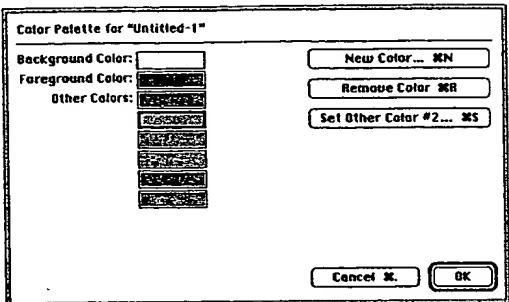
This section describes how to change the palette of colors available in the Color menu and the background color using the Color Palette dialog box in the File menu.

To change the palette of colors used in the current document:

- From the File menu, choose a Color Palette.

The Color Palette dialog box appears.

Figure 11-2 The Color Palette dialog box



The Background Color is used to fill the background of the current document in the active window. The Foreground Color is the default color used whenever you draw a new object. Other Colors are the colors available in the Color menu for changing the color of individual objects. The colors are represented in the same order that they appear in the Color menu. The Set button changes to reflect the color selected. For instance, if you select the second Other Color, the name of the buttons changes to Set Other Color #2. When you select either the foreground or background color, the button changes to Set Foreground Color, or Set Background Color.

To change a color in the color palette:

- Click the color you want to change.

A highlight box appears around the color, indicating that it is selected, and the Set Color button changes to the number associated with the color. For instance Set Other Color #2.

- Click the Set Color button or double-click the color.

The Color Wheel dialog box containing the Macintosh Color Wheel appears (in System 7.5, the Color Picker appears).

NOTE: For information about the Color Picker, see your System 7.5 user's guide.

The Color dialog box appears.

Figure 11-3 The Color dialog box (Windows)

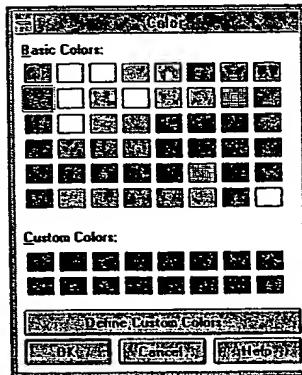
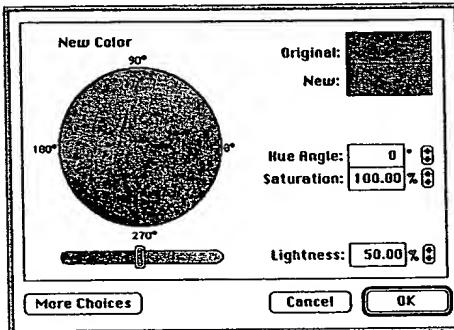


Figure 11-4 The Color Picker dialog box (Macintosh)



To specify a new color: (Windows)

- Click a color box in the Basic Colors section or the Custom Colors section.

A highlighted border appears around the color you select. To change to this new color:

- Click the OK button.

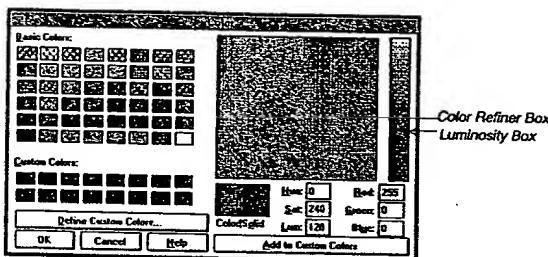
The color is changed to the new color and can be chosen from the Color menu of the active document window.

If, while in the Color dialog box, you do not find the color you want, you can create customized colors by doing the following:

- Within the Color dialog box, click the Define Custom Colors button.

The Color dialog box expands.

Figure 11-5 The Color dialog box when creating customized colors



The selected color appears in the left half of the Color/Solid box in the lower portion of the dialog box. You can change the hue, saturation, luminosity, and RGB components by changing the numbers in the boxes. You can also select a custom color by doing the following:

- Click a color in the Color Refiner box to set the hue and saturation.

The pointer turns into a Crosshair when you click. You can also hold the mouse button down and drag to a different region to change the hue and saturation.

- Next, click within the Luminosity box to set the brightness of the color.

When you have the color you want, click the Add button to add it to the Custom Colors.

To specify a new color: (Macintosh)

- Click a color in the Color Wheel.

The selected color appears in the upper half of Highlight Color Square, located in the upper left corner of the dialog box. The hue, saturation, brightness, and RGB components are listed on the left for the color that you have chosen. You can adjust the color by changing values within these boxes, in addition to, or instead of choosing from the Color wheel. For more information about the Macintosh Color Wheel, refer to your System documentation.

- Click the OK button.

The Color Wheel dialog box disappears and the newly selected color appears in the Color Palette dialog box replacing the color you originally clicked.

Adding Colors

To add a new color to the Color menu:

- Click the New Color button.

The Color dialog box appears.

- Click the color to add or create a customized color. Or, for the Macintosh, click a color in the Color Wheel.

The selected color appears in the upper half of Highlight Color Square, located in the upper left corner of the dialog box. The hue, saturation, brightness, and RGB components are listed on the left for the color that you have chosen. You can adjust the color by changing values within these boxes, as an alternate method from choosing from the Color wheel.

- Click the OK button in the Color Wheel dialog box.

The Color wheel dialog box disappears and the new color is added to the list of Other Colors.

Removing Colors

To remove a color from the Color menu:

- Click the color you want to remove.

A highlight box appears around the color.

- Click the Remove Color button.

The color disappears from the list of other colors.

To have all the changes take effect in the current document:

- Click the OK button in the Color Palette dialog box.

The Color Palette dialog box disappears. If you changed the background color, the background of the document is changed. If you changed the default foreground color, any object that was colored in the previous foreground color is now colored using the new foreground color. In addition, any new object you draw will also appear in the new foreground color. If you changed any of the other colors, objects previously drawn in those colors are changed to the new colors. If you removed a color, objects that were drawn in that color are changed to the Foreground color.

If you do not want any of the changes that you have made in the Color palette dialog box to take effect:

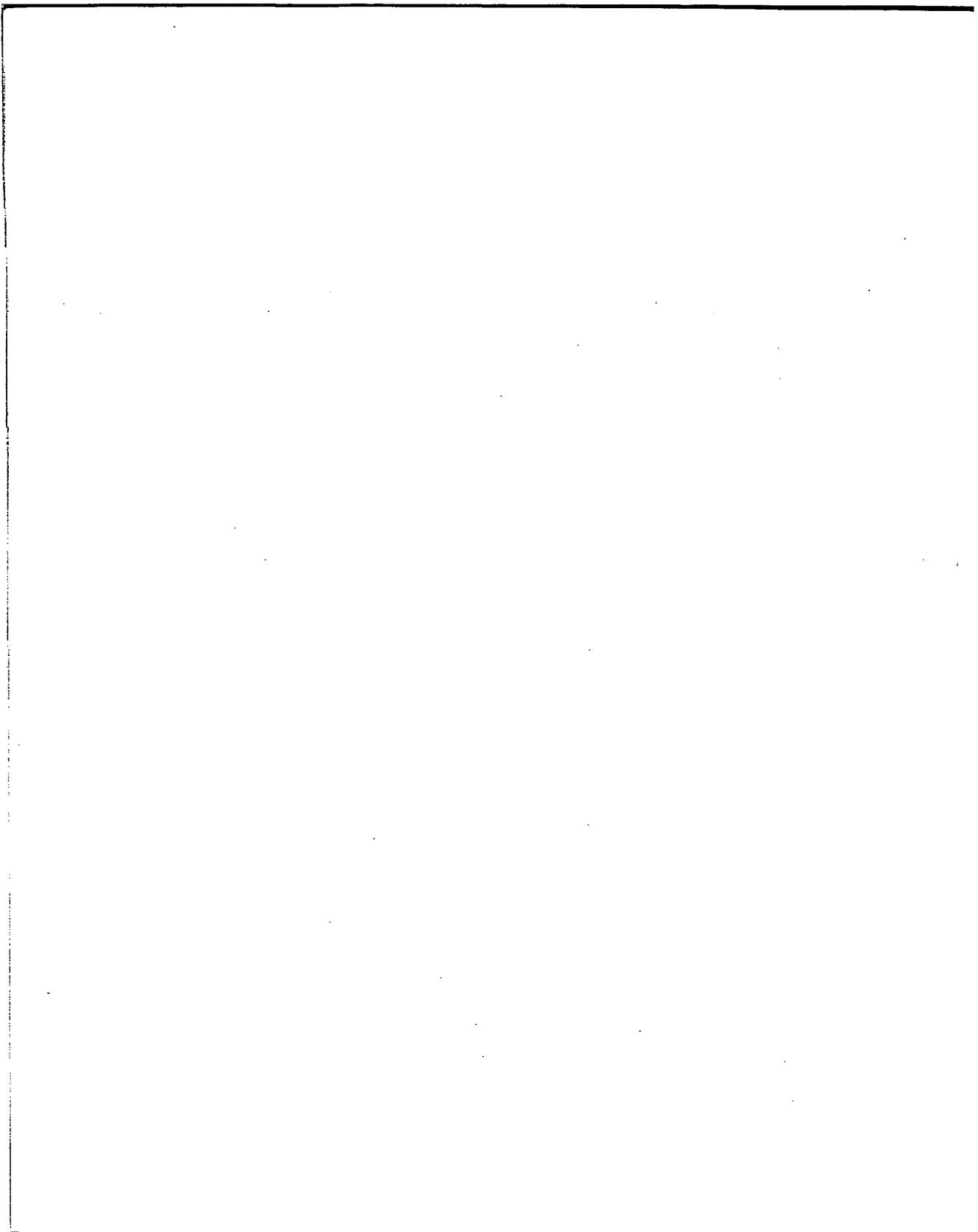
- Click the Cancel button in the Color Palette dialog box.

TEMPLATES AND COLOR

The background and foreground colors used in a template from the template pop-up palette are not used when the template is drawn in a document window. However, any other colors used in the template are added to the color palette of the current document if they are not already present. This is part of the autoscale feature. To learn more about autoscaling, see "Autoscaling" in *Chapter 13, Sharing Information*.

SAVING COLOR PALETTE SETTINGS

If you have customized the Color menu for a particular document that you know you will want to use again, you can save the Color Palette in a style sheet. The Color Palette is saved in addition to other document settings that you have made for the document such as Page Setup settings, Text settings, and Drawing settings. To learn more about saving settings in style sheets/stationery pads see "Saving Customized Settings" in *Chapter 1, ChemDraw Basics*.



Chapter 12, Working with Page Layout

The presentation quality of your *ChemDraw* document is determined by how well the chemical structures and other objects are placed on the page, also called the layout. Effective layout of a drawing includes proper alignment of chemical structures and other objects, appropriate page size, and page orientation. This chapter discusses the methods and tools available to achieve these ends, which includes setup of the page and the use of the ruler, Crosshair, grouping, layering, aligning, and distributing commands.

CONTROLLING THE DRAWING AREA

The size of a document window is not necessarily the same as the size of the drawing area of the page. A document window, in most cases, actually covers only a portion of the drawing area.

Enlarging the Drawing Area

To see more of the drawing area:

- Point to a border or corner of a document window and drag to resize. Or, for the Macintosh, drag the Size box in the lower right corner of the document window.

When the pointer is correctly positioned for resizing, the pointer changes to a multi-sided arrow (the direction of the arrowheads indicating the directions you can resize the window). You can enlarge a document window to a maximum size equal to the actual drawing area of the page (if the size of your monitor will accommodate this).

Scrolling within a Document Window

To move around the drawing area you can use the Scroll bars, Scroll boxes and Scroll arrows found on the right and bottom edges of a document window. You can scroll as far as the edge of the drawing area.

To view different sections of the drawing area in a document window:

- Click a Scroll arrow to move in small increments in that arrow's direction.
- Or, hold down the mouse button on a Scroll arrow to continuously scroll in that arrow's direction.
- Or, click in the gray area above/below or to the left/right of the Scroll box to move in large increments in that direction.
- Or, drag the vertical or horizontal Scroll box to move to the corresponding area of the drawing area.

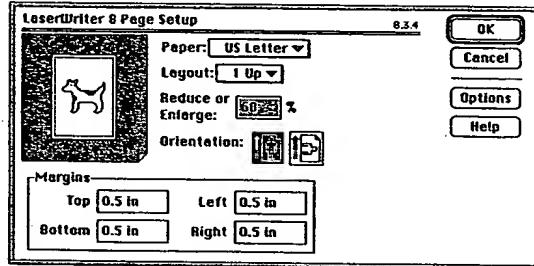
Page Setup

The parameters that affect the size and curve of the drawing area are the page size, orientation, and margins. These parameters are specified using the Print/Page Setup dialog box. The Print/Page Setup dialog box and the options available will vary depending on the printer you have chosen (and, for the Macintosh, the version of the printer driver for that printer installed in your System Folder.)

To set the paper size, orientation and margins:

- From the File menu, choose Print/Page Setup. The Print Setup dialog box appears. The dialog box will appear slightly different depending on the printer and platform you have.
- Select a page size.

Figure 12-1 Page Setup dialog box (Macintosh) showing common settings for a LaserWriter.



The available paper sizes vary depending on the type of printer. Listed below are common sizes available. The page orientation you choose will determine which of the measurements is height and which is width:

Table 12-1 Common paper sizes

US Letter	8.5 x 11 inches
US Legal	8.5 x 14 inches
A4 Letter	21 x 29.7 centimeters
B5 Letter	17.6 x 25 centimeters
Tabloid	11 x 17 inches
International	8.5 x 12 inches
Computer paper	14 x 11 inches

To choose a paper size:

- Select a paper size option/radio button.

Orientation

To choose the orientation of the page:

- Select the vertical (portrait) or horizontal (landscape) orientation button.

The orientation of a document window will change to the orientation you have chosen. This is evident when the rulers are visible.

Margins

To change the margins for the paper size you have chosen:

- Select the text next to the margin you want to change.
- Type the new margin measurement.

The units of the margins are set in the Preferences dialog box. The paper size minus the margins determines the drawing area.

- Click the OK button to exit with these changes.

NOTE: Most printers do not use other printers' Print/Page Setup settings; if you change printers (e.g., with the Chooser), you should check the Print/Page Setup settings for all of your documents.

Reduce or Enlarge

Some PostScript printers include an option to reduce or enlarge your drawings by a variable percentage (25-400%). This option will scale all objects and text in the document window by the percentage specified. This is not a change in magnification, which is discussed later in this chapter. The size of objects is changed relative to the paper size, margins, and orientation you have specified.

The enlarge or reduce option is useful for changing the size of the available drawing area, while keeping the images on the screen at the normal size when you are drawing. Another use for this option is if you have drawn structures to fill the area of the page specified using one printer, and then changed to another printer that requires larger margins; in this case your picture will seem to disappear off the edge of the page. You can reduce the size of the image using the reduce option and the picture will again appear in the document window.

Saving Settings

You can save Print/Page Setup settings in a style sheet/stationery pad. Whenever you open a style sheet/stationery pad, these settings are automatically used. The Print/Page Setup settings are saved in addition to the Text settings, Drawing Settings, and, the Color Palette. See "Saving Customized Settings" in *Chapter 1, ChemDraw Basics*, to learn more about using style sheets/stationery pads.

Footer

You can have a footer appear at the bottom left of your document window that contains the name of the document and the date and time it was last changed. The footer cannot be edited.

Preferences Guide

Include Footer

To have a Footer appear at the bottom of all *ChemDraw* documents:

- From the File menu, choose Preferences.
- Select the Include Footer check box.
- Click the OK button.

Changes to this preference will affect all documents.

35mm Slide Boundary Guides

If you are planning to make 35mm slides from a hard copy of a *ChemDraw* document, or by taking a screen shot, you can display boundary lines that appear on your screen positioned at 7 inches and 10.5 inches to match the 2:3 ratio for the 35 mm slide format. These guides help you keep your drawing within this region to maintain the proper ratio, but will not be printed. The drawing area of the page must be at least 7 x 10.5 inches for these boundary lines to be visible.

Preferences Guide

Show 35mm Slide Boundary Guides

To display the 35mm slide boundary lines:

- From the File menu, choose Preferences.
- Select the Show 35mm Slide Boundary Guides check box.
- Click the OK button.

Two 35mm Slide Boundary Guides appear in the same orientation you have chosen in the Print Setup dialog box. These guides will appear in every document.

Changes to this preference will affect all documents.

Changing Perspectives

Sometimes you may need to get a close-up view of certain objects in your reaction scheme, such as arrows and reaction mechanism symbols, to make sure that objects are properly positioned. At other times, you may want to reduce your view so that you can move groups of objects around the page. You can increase and decrease the magnification for performing these functions using the Magnify and Reduce commands in the Tools menu.

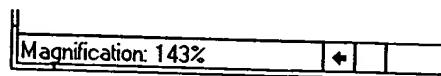
Magnify

To magnify the view on an object:

- Select the object around which you want to magnify your view.
- From the Tools menu, choose Magnify.

The magnification occurs around the center of the selected object. The magnification appears in the Message area of a document window. You can continue to magnify your view three more times to a maximum of 400%.

Figure 12-2 Message Area displaying a magnification



The last object drawn will be the center point of the magnification if you do not select an object in a document window.

Actual Size

To return to the actual size from any other magnification:

- From the Tools menu, choose Actual Size.

The view is returned to the original size. The Message area is empty.

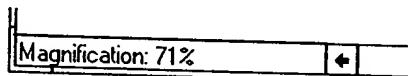
Reduce

To reduce the magnification:

- Select an object around which you want to reduce the magnification.
- From the Tools menu, choose Reduce.

The reduction in magnification appears in the Message area of the document window.

Figure 12-3 Message Area displaying a reduction



You can reduce the magnification until the entire page fits on the screen. The size of your monitor will determine the low end for this reduction. For instance, you can reduce the magnification in one increment to 71%, on a 16 inch monitor, whereas you can reduce the magnification in three increments to 35%, on a 9 inch monitor.

In the reduced view, you can continue to use all of the drawing tools. In particular, you can use the Selection tool to rearrange the drawing in order to take better advantage of the space available.

Show Page

The Show Page command is equivalent to repeatedly choosing the Reduce command until the entire page is visible in the document window.

To view the entire drawing area in a document window at once:

- From the Tools menu, choose Show Page.

The Message area shows the reduction in magnification that was required to have the entire page appear on the screen. This magnification also reflects the minimum magnification that you can obtain using the Reduce command.

ARRANGING OBJECTS

This section describes methods for positioning, aligning, and layering objects in a document window.

Using Rulers

You can use the rulers to position objects a measured distance away from some reference point or create objects of an approximate size. The units used for the ruler are set in the Preferences dialog box, where you have the choice of inches, centimeters or points.

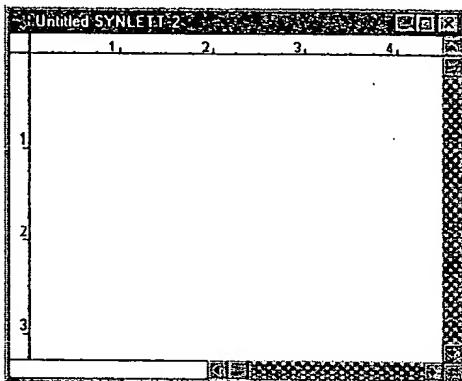
Show Rulers

To display the rulers:

- From the Tools menu, choose Show Rulers.

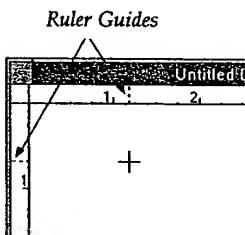
A check mark appears next to the Show Rulers command, and the rulers appear along the top and left edges of a document window.

Figure 12-4 Rulers in a document window



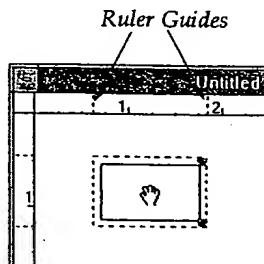
As you move the pointer, **Ruler Guides** appear on each ruler, indicating the position of the pointer.

Figure 12-5 Ruler guides when pointing



Ruler guides also appear when you drag selected objects. In this case, however, there are two Ruler guides that bracket the object. With this bracketing you can quickly establish the height and width of the selected object(s).

Figure 12-6 Ruler Guides when moving a selection



Hide Rulers

To Hide the rulers:

- From the Tools menu, choose Show Rulers.

The check mark disappears.

Using the Crosshair

You can use the Crosshair to align objects relative to each other, and to space objects a consistent distance apart. The axes of the Crosshair can be moved within a document window.

Show Crosshair

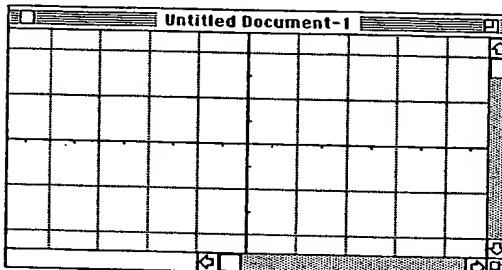
To show the Crosshair:

- From the Tools menu, choose Show Crosshair.

A check mark appears next to the Show Crosshair command and the Crosshair appears within a document window.

To assist you in aligning objects, the Crosshair includes grid lines which extend from the major division marks on each Crosshair axis.

Figure 12-7 The Crosshair



You can also show the Rulers while the Crosshair is displayed so that you can see the unit measurement associated with each of the divisions on the Crosshair axes.

Moving the Crosshair

To move the Crosshair:

- Position the pointer where the Crosshair axes intersect.

When the pointer is near to the center of the Crosshair, it changes to an arrow.

- Drag the Crosshair.

To constrain the movement of the Crosshair to the X or Y direction:

- Alt+drag (Windows) or Command+drag (Macintosh) the Crosshair.

Aligning Objects using the Crosshair

To use the Crosshair to align objects:

- Move the Crosshair axes and align it with the object.
- Or, select an object and drag it until it is aligned with either axis of the Crosshair, or a grid line.

In either case, if a bond or side of the object is parallel to one of the axis, it will disappear when it is exactly positioned over a Crosshair axis.

To align another object on the Crosshair.

- Select a second object.

- Drag the second object to the Crosshair axis or grid line and align it to the first.

You can also move selected objects in small increments to align them with the Crosshair using the Arrow keys available on some keyboards:

To move 1 point in the direction of an Arrow key (1 point equals 1/72 inch, or 0.035 cm):

- Select the object(s) and then press an Arrow key.

To move 10 points using the Arrow key, for example, to the right:

- Press **Ctrl+Right Arrow (or Option+Right Arrow)**.

Hide Crosshair

To hide the Crosshair:

- From the Tools menu, choose Show Crosshair.

The checkmark next to the Show Crosshair command disappears.

Centering on a Page

To center an object (or group of objects) at the center of the page:

- Select the object you want to center using the Selection tool.
- From the Object menu, choose Center on Page.

The selected objects move so that the center of the Selection rectangle is positioned at the center of the page.

Aligning Objects

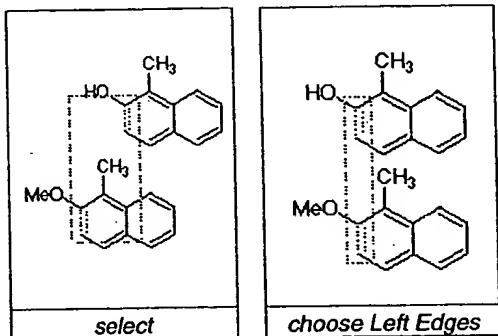
There are several align commands available in the Align submenu from the Object menu. Choose any of these commands to align objects relative to each other.

To align two or more objects:

- Select the objects with the Selection tool.
- From the Align submenu, choose one of the Align commands.

If you select only part of a structure or group with the Selection tool, only that part is used for the alignment operation, but the entire structure or group is moved.

Figure 12-9 Aligning structures



Distributing Objects

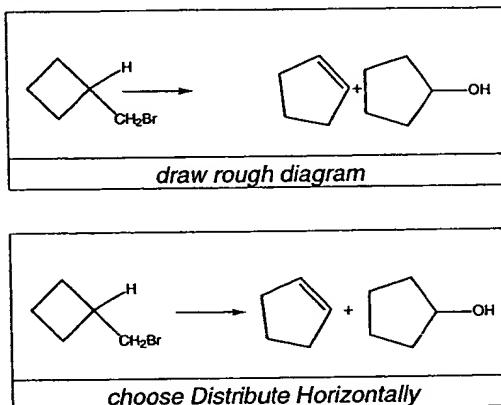
There are two distribute commands available in the Distribute submenu in the Object menu. Choose one of these commands to distribute objects horizontally or vertically and an equal distance apart. In combination with the align command, you can easily clean up the appearance of a reaction.

To distribute 3 or more objects:

- Select the 3 or more objects to distribute.
- From the Distribute submenu in the Object menu, choose Vertically or Horizontally.

The space between the objects is equalized. The position of objects in your selection that are rightmost and leftmost (or uppermost and lowermost) remain unchanged.

Figure 12-10 Spacing structure evenly along the x-axis



Front to Back Ordering

The front to back ordering is a useful method for changing the orientation of one object relative to another object within the same picture layer. For additional information specific to the layering of bonds, see "Bond Crossings" in Chapter 3, *Drawing Chemical Structures*.

Picture Layers

There are three layers within a *ChemDraw* document. From back to front, they are: imported pictures, graphical *ChemDraw* objects and text. The ordering of these layers cannot be changed. However, the front to back ordering of objects within each layer can be specified with the Bring to Front and Send to Back commands in the Object menu.

For example, if an imported picture is dragged onto a *ChemDraw* structure, the structure will not be hidden since the imported picture resides in the backmost layer.

An imported picture is any picture pasted into a *ChemDraw* document from another application such as a molecular model or a graph from a graphing application. The picture can be imported into the *ChemDraw* document by using the Paste command. A graphical *ChemDraw* object is any structure or object created within *ChemDraw*, excluding text. Text, including both atom labels and captions, is always the frontmost layer.

NOTE: When you point at an imported picture, a highlight box appears around the periphery of the object that helps distinguish it from a graphical *ChemDraw* object. Text also has this type of highlight box

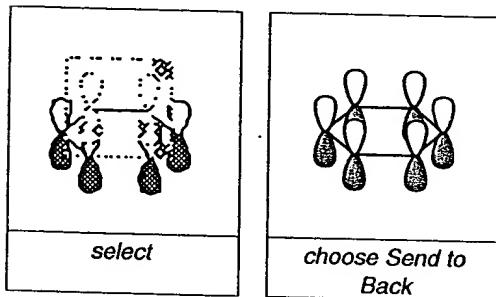
Send to Back

To place one object behind another within a layer:

- Select the object that you want to send to the back.
- From the Object menu, choose Send to Back.

The selected object appears behind all other objects in the same layer.

Figure 12-11 Changing layering of p-orbitals



Bring to Front

To place one object in front of another within a layer:

- Select the object that you want to move forward.
- From the Object menu, choose Bring to Front.

The selected object now appears in front of all other objects in the same layer.

Chapter 13, Sharing Information

This chapter describes several ways to transfer information between *ChemDraw* and other applications. *ChemDraw* includes many of the standard system commands for transferring information within *ChemDraw* documents, between *ChemDraw* documents and between documents created using other applications via the Clipboard, drag and drop, object embedding and file formats.

WORKING BETWEEN CHEMDRAW DOCUMENTS

You can use the Clipboard or Drag and Drop to transfer *ChemDraw* pictures to other *ChemDraw* documents.

Copy

To place a *ChemDraw* picture on the Clipboard:

- Select the objects to copy using the Selection tool.
- From the Edit menu, choose Copy.

A copy of the selected objects is placed on the Clipboard. The selected objects in a document window remain unchanged.

Cut

To place a copy of the *ChemDraw* objects on the Clipboard and remove the objects from a document window:

- Select the objects to remove using the Selection tool.
- From the Edit menu, choose Cut.

A copy of the selected objects is placed on the Clipboard. The selected objects are removed from a document window.

Paste

To paste the contents of the Clipboard into a *ChemDraw* document window:

- From the Edit menu, choose Paste while the Selection tool is selected.
- The contents of the clipboard are placed in the center of the active document.

If the Clipboard contains *ChemDraw* structures, the pasted information is scaled to the settings in the current document. See "Autoscaling" in this chapter for more information.

To view the contents of the Clipboard:

- Return to the Program Manager or File Manager and start the Clipboard Viewer. Or, for the Macintosh, choose Show Clipboard from the Edit menu.

Refer to your operating system documentation for information on using the Clipboard.

NOTE: You can paste the contents of the Clipboard into another application by the same procedure. Refer to your application documentation for additional information specific to the application. Macintosh: If you are pasting the *ChemDraw* picture in a document from which you are planning to print to a PostScript printer, refer to the section "Including PostScript" later in this chapter for important information.

Drag and Drop

Another way to copy information between *ChemDraw* documents and other applications' documents is through drag and drop. This feature provides streamlined copy and paste that bypasses the Clipboard.

NOTE: If you are using the Macintosh version and have system software prior to System 7, you will need the Drag and Drop extension loaded for this to work.

To copy and paste information between *ChemDraw* documents using Drag and Drop:

- Select an object or structure in a *ChemDraw* document.
- Drag the selection into another *ChemDraw* document window.

The selection is copied to the destination *ChemDraw* document.

To copy and paste a selection to another application's document:

- Select an object or structure in a *ChemDraw* document.
- Drag the selection into another application's document window.

The selection is copied to that application's document.

NOTE: *The other application, like ChemDraw, must support Drag and Drop for this feature to work.*

Using Drag and Drop, you can also create clipping files (Macintosh) or scrap files (Windows 95 only).

To create a clipping file or a scrap file:

- Select an object or structure in a *ChemDraw* document.
- Drag the selection out of the *ChemDraw* document window onto the desktop.

A clipping file or a scrap file is created on your desktop.

NOTE: *(Macintosh only) You must have the Clipping Extension installed to create a clipping file if you are using system software prior to 7.5.*

To view the information within a clipping file or a scrap file:

- Double-click the file's icon.

A window appears showing the *ChemDraw* picture. Click the close box to close the clipping file's window.

To use the contents of a clipping or scrap file in a document:

- Drag the clipping or scrap file into an open window of an application that supports Drag and Drop, such as an open *ChemDraw* document window.

The contents of the clipping or scrap file are copied to the open window. The clipping or scrap file remains unchanged.

Autoscaling

When you transfer *ChemDraw* objects via the Clipboard or drag and drop from one *ChemDraw* document (the source document) to another *ChemDraw* document (the destination document), the objects are scaled to match the document settings of the destination document. This automatic scaling assures that the objects being transferred will match the settings of the current document.

Bonds

All bonds drawn in the source document using the values specified in the Drawing Settings dialog box will be changed to use the Drawing Settings in the destination document.

Any bond that has been resized in the source document will be scaled in the destination document. The scale factor used is based on the ratio of the bond's length after resizing (source) to the Fixed Length in the Drawing Settings dialog box (source). This scaling process maintains the proportions in the destination document that are present in the source document. All values in the Drawing Settings dialog box are scaled in this same manner.

For example, in a source document, the Fixed length is set to 1.0 cm. A benzene ring is resized in the source document to 200%, so the bond length is actually 2.0 cm, which represents a ratio of 2.0 cm / 1.0 cm or a scale factor of 2. A destination document has a fixed length set at 1.7 cm. When the benzene ring is pasted into the destination document, the bonds will be scaled by a factor of 2 to a final bond length of 3.4 cm.

Atom Labels

Atom labels are scaled in the same fashion as bonds discussed in the previous section.

For example, the atom label font size is set to 16 points in Label Text Settings dialog box of the source document. One or two atom labels in the source document are resized to 8 points, which represents a ratio of 8/16 or a scale factor of 0.5. The destination document has an atom label font size of 14 points set in the Label Text Settings dialog box. When the atom label is pasted into the destination document, the font size is scaled by a factor of 0.5 to give a final atom label font size of 7 points.

Captions

Captions are always autoscaled based on the ratio of the fixed length in the destination document to the fixed length in the source document times the caption font size (the font size of the caption can be any size and is not related to the setting in the Caption Text Settings dialog box, as discussed for atom labels). This assures that captions are always in proportion to the bonds with which they are pasted.

For example, If the source document has a fixed length of 1.0 cm and the destination document has a fixed length of 2.0 cm, and the caption you are pasting is 12 points, then the resulting caption size after autoscaling is $(2.0 \text{ cm} / 1.0 \text{ cm}) \times 12 \text{ points} = 24 \text{ points}$.

Non-bond Objects and Color

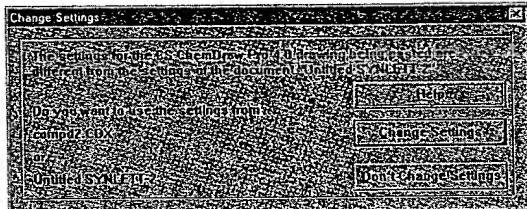
All objects that are not affected by settings in the various Document Settings dialog boxes, such as arrows, boxes and so on, will be scaled to maintain the same proportions to bonds that were present in the source document.

With the exception of the foreground and background color, the other colors present in the selection to be pasted are added to the destination document's Color Palette if they are not already present (up to a maximum of 20 total colors). The background color in the destination document remains unchanged, and all objects colored using the foreground color are changed to match the foreground color in the destination document.

Pasting to an Empty Document Window

If you are pasting a ChemDraw drawing to an empty ChemDraw document, and the settings between the documents are different, the following dialog box appears:

Figure 13-1 Change Settings dialog box



To change the settings in the destination document to match the settings in the source document:

- Click the Change Settings button.

All of the settings in the various document settings dialog boxes in the destination document (the document being pasted to) are changed to match those of the source document (the document from which it is being copied). All of the colors in the Color Palette of the destination document, including the Foreground and Background color are changed to those specified in the source document.

To scale the objects from the source document to the settings in the destination document:

- Click the **Don't Change** button.

The settings from the source document (the document being copied from) are scaled to those in the destination document (the document being copied to) using the ratios discussed previously.

NOTE: If the source document was created in a version of ChemDraw that is earlier than version 3.0, the name of the document will appear as "Unknown" in the dialog box.

EMBEDDING OBJECTS

For making changes to ChemDraw pictures that are pasted in other types of documents, ChemDraw supports the Object Linking and Embedding (OLE) protocol on Windows and the Edit Graphics Objects (EGO) protocol on the Macintosh.

NOTE: ChemDraw running under Windows is an OLE server, which means it can create OLE objects that can be copied and pasted into other OLE client applications.

OLE (Windows Only)

When a picture is transferred from ChemDraw into another type of document that supports OLE, you can open the picture (often by double-clicking it) and the picture appears in a ChemDraw document window. Any changes you make within the ChemDraw document window are automatically reflected in the other document when you close the ChemDraw window.

For example, to edit a ChemDraw picture pasted into Microsoft Word for Windows version 6.0 or later.

- Double-click the **ChemDraw picture that is pasted into a Microsoft Word document**.

The ChemDraw application will launch if it is not already running. The picture opens in a window titled "From Microsoft Word". You can use all the tools available in ChemDraw to edit the picture. When you have finished making changes:

- From the File menu, choose close.

The ChemDraw document window disappears and the picture in the Microsoft Word document is updated with any changes you made.

EGO (Macintosh Only)

When a picture is transferred from ChemDraw into another type of document that supports the EGO protocol, you can open the picture (often by double-clicking it) and the picture appears in a ChemDraw document window. Any changes you make within the ChemDraw document window are automatically reflected in the other document when you close the ChemDraw window.

NOTE: By including the "EGO for Word" file supplied with ChemDraw in the Word Commands folder, Microsoft Word™ version 5.x. EGO is not supported in Word 6.0 for the Macintosh. Other applications such as WordPerfect 3.x, FullWrite and ClarisWorks supports the EGO protocol without the use of extensions.

For example, to edit a ChemDraw picture pasted into Microsoft Word (version 5.x only for the Macintosh):

- Double-click the **ChemDraw picture that is pasted into a Microsoft Word 5.x document**.

The ChemDraw application will launch if it is not already running. The picture opens in a window titled "From Microsoft Word". You can use all the tools available in ChemDraw to edit the picture. When you have finished making changes:

- Click the Close box in the **ChemDraw document window**.

The ChemDraw document window disappears and the picture in the Microsoft Word document is updated with any changes you made.

NOTE: All colors, except for the Background Color, are transferred with a ChemDraw picture pasted into another document type. The Background Color is always removed.

(Macintosh only) You can also edit pictures within *ChemDraw* that are pasted from other applications that also support EGO. CS *Chem3D* is one such application.

To edit a picture that is pasted into a *ChemDraw* document from another application's document that supports EGO:

- Double-click the picture using the Selection tool.

A document window from the application that created the picture appears with the contents of the picture. All of the tools and commands used to create the picture are available for editing the picture. The title bar of the document window may read "From Application Name" indicating the application where the picture being edited resides.

NOTE: In applications such as *ChemDraw* and CS *Chem3D*, you can display the location of the document that the picture being edited resides by holding down the Command key and pressing the mouse button while pointing at "From Application Name" in the title bar.

For example, to edit a CS *Chem3D* picture pasted into *ChemDraw*:

- Double-click the *Chem3D* picture using the Selection tool.

The CS *Chem3D* application will open if it is not already running. The picture opens in a *Chem3D* Model window titled "From *ChemDraw*". You can use all of the tools available in CS *Chem3D* to edit the picture.

When you have finished making changes:

- Click the Close box in the *Chem3D* Model window.

The CS *Chem3D* Model window disappears and the picture in the *ChemDraw* document is updated with any changes you made.

Transferring PostScript (Macintosh only)

To obtain the highest quality drawings possible on a PostScript printer, *ChemDraw* creates both a screen representation and a PostScript representation of your drawing. PostScript is a page-definition language used to describe pictures. Many printers, including most Apple LaserWriter printers, use PostScript to create high quality output.

The PostScript representation of a *ChemDraw* picture is composed of two parts, the PostScript commands and the *ChemDraw* Laser Prep. The *ChemDraw* Laser Prep contains specific instructions that enable the laser printer to interpret the PostScript commands contained in a *ChemDraw* document.

If you are transferring a *ChemDraw* picture to another application on the Clipboard, through an edition file, using EGO, or through EPS files you need to specify that both the PostScript commands and the *ChemDraw* Laser Prep be sent along with the picture. You can specify this in the Preferences dialog box. There are several different situations that require either one or both to be selected.

Preferences Guide (Macintosh)

Include PostScript; Include ChemDraw Laser Prep

If you are transferring several pictures to other applications and you also have access to *ChemDraw*.

- From the File menu, choose Preferences
- Select Include PostScript and deselect Include ChemDraw LaserPrep.

To print the document(s):

- Choose Initialize LaserWriter from the File menu within *ChemDraw*.

This command sends the *ChemDraw* Laser Prep directly to your printer. You do not need to send this command for each document you are printing, since the *ChemDraw* Laser Prep remains in the printer's memory until the printer is turned off or reinitialized.

If you are transferring only a few pictures to another document, or if you are transferring pictures to a document in a remote location whose printer cannot be initialized by *ChemDraw*:

- Select **Include PostScript** and **Include ChemDraw Laser Prep** in the Preferences dialog box.

In this instance both the PostScript commands and the *ChemDraw* Laser Prep are transferred with each picture. *ChemDraw* pictures transferred in this manner can be printed independently of *ChemDraw*. The *ChemDraw* Laser Prep file adds approximately 11K to 12K to the size of each picture.

If you do not check the **Include PostScript** checkbox when printing to a PostScript printer *ChemDraw* sends QuickDraw commands to the printer. See "Print Quality" in *Chapter 1, ChemDraw Basics*, for more information about QuickDraw.

If you do not have access to a PostScript printer, or you are printing to a non-PostScript printer, or you are transferring *ChemDraw* pictures to a drawing program that does not use PostScript commands (such as a Paint program):

- Deselect both **Include PostScript** and **Include ChemDraw Laser Prep** in the Preferences dialog box.

For best print quality under all circumstances (at the expense of slightly larger files) you are encouraged to check both the **Include PostScript** and **Include ChemDraw Laser Prep** preferences. This will give you the greatest flexibility if you give your document to someone else or later want to print it on a PostScript printer.

Publishers, Subscribers, and Editions (Macintosh only)

This section describes how to share information through a dynamic link between a *ChemDraw* document and one or more other application documents using the publish, subscribe and edition features. For example, you can link a *ChemDraw* document to another *ChemDraw* document and also to a word processing program.

To create a link, you designate a portion of a *ChemDraw* document as a publisher and save a picture of the publisher in an edition file. You can then designate an area within a document as a subscriber and also link to this edition file. Changes made to the publisher will update the edition file, which in turn will update the subscriber. Updating can be automatic or manual depending on the options you choose. The subscriber document does not need to be open for this updating process to occur, as updating is done in the background.

NOTE: All colors, except for the Background Color, are contained within an edition file. The Background Color is always removed.

NOTE:  In *ChemDraw Pro*, you cannot publish or subscribe from a Template document.

Creating a Publisher

To create an edition file, you first need to identify the part of your *ChemDraw* document that you want to publish:

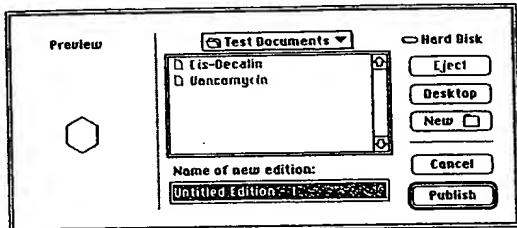
- Select the objects(s) to publish using the Selection tool.

To specify where to create the edition file containing a picture of the selected objects:

- From the Edit menu, choose Create Publisher

The Create Publisher dialog box appears where you can specify the name of the edition file, and the folder and disk where you want to place the file.

Figure 13-2 Create Publisher dialog box

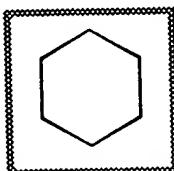


The Create Publisher dialog box is the same as the Save File dialog box with the addition of a Preview section on the left side. A picture of the portion of the document that you are publishing appears in the Preview section.

- Type a name for the edition file, and choose a folder to save it in.
- Click the Publish button.

The Create Publisher dialog box disappears. The object you selected is enclosed in a gray rectangle called a Publisher border.

Figure 13-3 A cyclohexane structure enclosed in a publisher border



The entire area contained within the borders of the publisher is included in the edition file. Any object or part of an object that is inside the borders of the publisher will appear in any document that subscribes to the edition file. The publisher border is an object; and so it can be selected, moved and resized independent of its contents, using the Selection tool.

To resize a publisher border without changing its height to width ratio:

- Select the publisher border by clicking with the Selection tool.
- Drag the resize handle on the Resize handle.

To resize a publisher border in the X or Y direction only:

- Hold down the Command key and drag the Resize handle.

When the edition file is updated, the two carbons of the cyclopentane ring will appear in any document that subscribes to the edition file.

Publisher borders appear only on the screen. They are not printed.

To hide the Publisher borders:

- From the Edit menu, choose Show Borders.

The checkmark disappears as well as the publisher border.

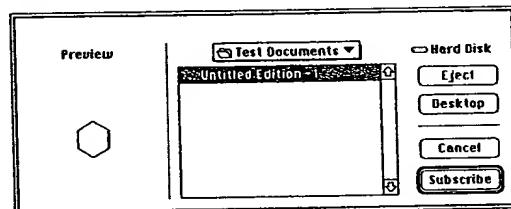
Subscribing to an Edition File

To subscribe to the contents of an edition file:

- From the Edit menu, choose Subscribe To.

The Subscribe To dialog box appears where you can select the edition file to which you want to subscribe.

Figure 13-4 Subscribe To dialog box



The Subscribe To dialog box is the same as the Open File dialog box with the addition of a Preview section on the left side.

- From the directory listing, select the edition file you want to subscribe to.

A picture of the contents of the edition file appears in the Preview section.

- Click the Subscribe button.

The Subscribe To dialog box disappears. The most recent edition appears in the document window enclosed in a gray rectangle called a **Subscriber border**.

A subscriber is an object that can be selected, moved and resized using the Selection tool. If you resize a subscriber, each time an edition file is updated the contents will appear resized. The Subscriber border appears only on the screen. It is not printed.

To hide the Subscriber borders:

- From the Edit menu, choose Show Borders.

The checkmark disappears as well as the subscriber border.

Publisher Options

You can use the Publisher Options command to specify when an edition file is updated with changes made to the publisher and to display other information about the edition file.

To open Publisher Options:

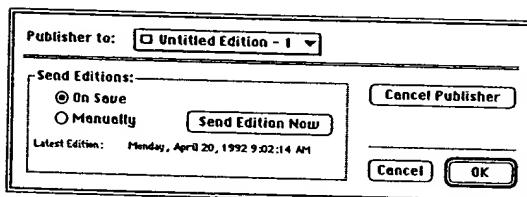
- Select a publisher by clicking the Publisher border using the Selection tool.
- From the Edit menu, choose Publisher Options.

or

- Double-click the Publisher border.

The Publisher Options dialog box appears.

Figure 13-5 Publisher Options dialog box



Publisher to

To display a pop-up menu listing the location of the edition file linked to the publisher:

- Point to the Publisher to pop-up menu and hold down the mouse button.

Send Editions

You can specify when a publisher sends a new edition to an edition file by setting options within the Send Editions section. In *ChemDraw*, each time a publisher updates an edition file, the edition file contains the most up-to-date picture of the object(s) contained within the publisher border.

To update an edition file automatically each time the document is saved:

- Select the On Save radio button.

By using this option you do not need to remember to send updates every time you make changes to objects contained within the Publisher border.

To have more control over which revisions of the publisher will be sent to the edition file:

- Select the Manually radio button.

To update the edition file when the Manually radio button is selected:

- Click the Send Edition Now button.

The Latest Edition is the last date and time the edition file for the publisher was updated. When the Manually radio button is selected, the Last Change appears below the Latest Edition time and refers to the last date and time that changes were saved in the edition file.

Cancel Publisher

To delete a publisher and its corresponding edition file:

- Click the Cancel Publisher button.

An alert appears asking you if you are sure that you want to remove the selected publisher. When you cancel a publisher, the publisher border around the picture is removed from the document. The edition file is deleted when the document is saved.

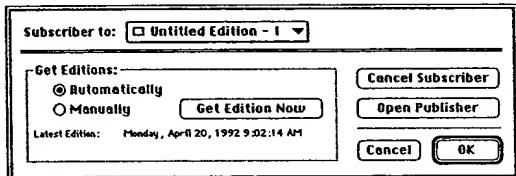
Subscriber Options

You can use the Subscriber Options command to specify when a subscriber is updated with the contents of the edition file.

- Click the **Subscriber border** using the Selection tool.
- From the **Edit menu**, choose **Subscriber Options**.
- Or, double-click the **Subscriber border**.

The Subscriber Options dialog box appears.

Figure 13-6 Subscriber Options dialog box



Subscriber to

To display a pop-up menu showing the location of the edition file linked to the subscriber:

- Point to the **Subscriber to** pop-up menu and hold down the mouse button.

Get Editions

You can specify when a subscriber receives the updated edition by setting the options within the Get Editions section.

To update the subscriber automatically each time the document is opened and each time the edition file is updated:

- Select the **Automatically** radio button.

To specify each time the subscriber will be updated with the most recent version of the edition file:

- Select the **Manually** radio button.

To update the subscriber when the Manually radio button is selected:

- Click the **Get Edition Now** button.

The **Latest Edition Time** is the last date and time that the edition file for the selected subscriber was updated. When the Manually radio button is checked the **Last Received** time appears below the last edition time. The Last Received time is the date and time the contents of the edition file were used to update the subscriber.

Open Publisher

To open the document containing the publisher:

- Click the **Open Publisher** button.

Cancel Subscriber

To break the connection between the selected subscriber and the edition file:

- Click the **Cancel Subscriber** button.

An alert appears asking you if you are sure that you want to remove the selected subscriber. When you break the connection, the subscriber will be removed, but the picture will remain in your document.

The Edition File

To display the contents of an edition file:

- Select the **edition file icon** in the **Finder**.

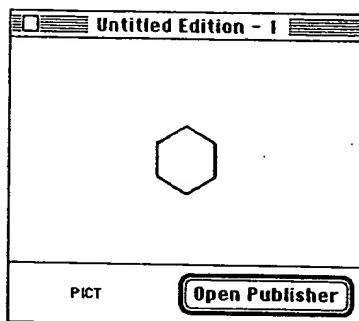
Figure 13-7 Edition file icon



- From the **File menu**, choose **Open**, or double-click the icon.

A window appears containing a picture of the contents of the edition file.

Figure 13-8 Window containing contents of edition file



NOTE: The word in the lower left corner refers to the type of information contained within the edition file, in this instance it is PICT.

Open Publisher

To open the document containing the publisher linked to this edition file:

- Click the Open Publisher button.

IMPORTING AND EXPORTING

There are two ways to transfer *ChemDraw* pictures to and from other applications: using different file formats, and using the Clipboard. File formats are useful for saving and opening the contents of a *ChemDraw* document for transfer to other chemistry, word processing and desktop publication applications on the same or a different computer. Example output files for chemistry file formats are shown in the on-line help file under the topic "Chemistry File Formats". The Clipboard, as discussed earlier, is useful for transferring part or all of the information within an active document window between applications on the same computer or a networked computer. In *ChemDraw Pro*, the Clipboard is extended for use in transferring information to other chemistry applications as SLN strings, SMILES strings and in ISIS format.

Exporting via the Clipboard

It is common to copy structures to the Clipboard for pasting into another chemistry application for further analysis or storage. To assist in the process, *ChemDraw* includes several formats on the Clipboard during a normal copying operation. Below are the supported by *ChemDraw*'s Clipboard.

ChemDraw 4.0 (*.cdx)
ChemDraw 3.5 (*.chm)
PICT (Macintosh only)
WMF (*.wmf, Windows only)
PostScript (Macintosh only with appropriate preferences turned on)
ISIS/Sketch (SKC)
MDL Molfile (when no arrow is in the selection)
RXN File (when an arrow is in the selection)
DARC F1

Each of these formats is briefly described in the next section under file formats. In addition, Chapter 9, *Drawing Query Structures* includes some additional information as to what information is and is not copied.

To export a file using the Clipboard:

- Select the structure using the Selection tool.
- From the Edit menu, choose Copy.

The structure is copied to the Clipboard. For large structures you may see a status bar indicating the progress.

In addition, you can choose one of several commands for created text string representations of selected structures that are copied to the Clipboard. These include SMILES and SLN strings.

Creating SMILES Strings

A SMILES string is a way of describing a chemical structure in a line of text, similar to the Wiswesser Line Notation used many years ago. Several software packages use SMILES strings as a compact means of entering and storing chemical structure information.¹

For example, to create the SMILES string for the following structure:

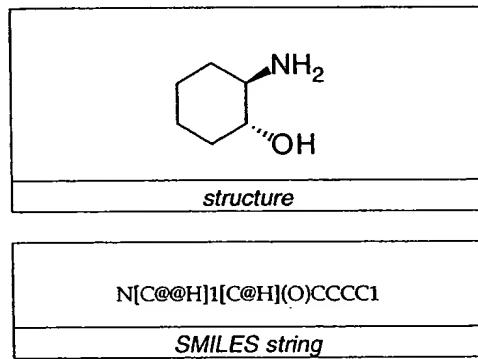
- Select the structure using the Selection tool.
- From the Copy As submenu in the Edit menu, choose SMILES.

The SMILES string corresponding to the *trans*-2-amino-cyclohexanol molecule is transferred to the Clipboard.

To display the SMILES String:

- Switch to the Program Manager or File Manager and start the Clipboard Viewer.

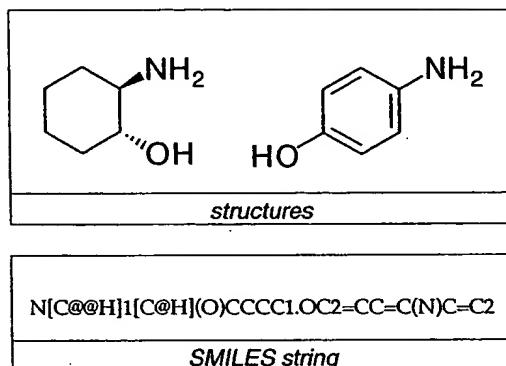
Figure 13-9 Converting a structure into a SMILES strings



Once the SMILES string is on the Clipboard, you can transfer it to another application that can interpret and manipulate SMILES strings.

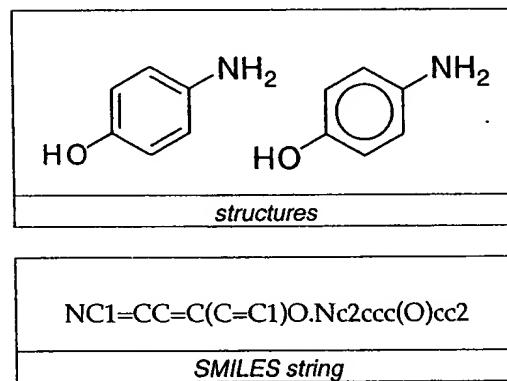
If you select more than one structure in *ChemDraw*, and choose Copy SMILES from the Edit menu, the SMILES string for each structure will be copied to the Clipboard and separated from the previous SMILES string by a period.

Figure 13-10 Converting two structures into SMILES strings



SMILES supports an alternate notation for aromatic structures using lowercase letters. *ChemDraw* will generate this type of SMILES string for any structure drawn with explicit aromatic bonds, either by using the Aromatic bond type in the Atom Properties dialog or by placing a circle within any ring structure

Figure 13-11 Alternative notation for aromatic structures



PRO Paste SMILES via Clipboard

If you have a SMILES string, a way of describing a chemical structure in a line of text, then you can automatically convert that text string into a *ChemDraw* structure.

- Select the SMILES string using the Text tool.
- From the Edit menu, choose Copy.
- From the Paste Special submenu in the Edit menu, choose SMILES.

Your SMILES string is drawn as a structure.

NOTE: Paste SMILES uses the same routines as the Clean Up structure command. For more information about this command see "Structure Clean Up".

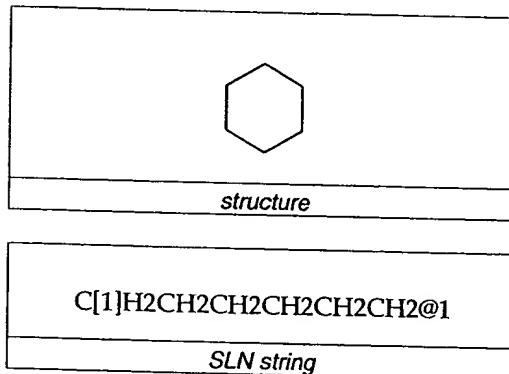
PRO Creating SLN Strings

Similar to creating a SMILES string, you can copy a *ChemDraw* structure to the Clipboard as an SLN string for export to a TRIPPOS application.

- Select a structure.
- From the Copy As submenu in the Edit menu, choose SLN.

The Structure is copy to the clipboard as an SLN String.

Figure 13-12 Cyclohexane structure and the resulting SLN string on the Clipboard



EXPORTING AND IMPORTING USING FILE FORMATS

Many applications can use the information contained within a *ChemDraw* document that has been saved in one of the other file formats provided with *ChemDraw* or *ChemDraw Pro*. File formats are available in a pop-up menu (drop-down list) at the bottom of the Open and Save dialog boxes. This section briefly discusses the formats that are available.

To export a file:

- From the File menu, choose Save As.

In the Save As dialog that appears do the following:

- Type a name for the file and choose a location in which to save it.
- Select a file format from the bottom of the dialog box.
- Click the OK (Windows) or Save button (Macintosh).

A copy of the current document is saved in the format you specified. The current document remains unchanged.

This remainder of this section briefly (in alphabetical order) discusses the formats that are available.

NOTE: Some file formats do not support atom labels that contain nicknames (Me, Ph) or structural fragments (CH₂CH₂CH₃, COOH). When saving in these formats, *ChemDraw* automatically expands all atom labels (see "Expand Label" in Chapter 8, Advanced Drawing Techniques, for more information) and saves the file using the expanded form. The following formats are affected in this way:

Connection Table
DARC F1
DARC F1 Query
MDL MolFile
MSI MolFile
ISIS RXN
SMD

CD Template (*.ctp, *.ctr)

The CD Template file format is used for saving template documents that will appear in the template pop-up menu (when stored in the cd_items directory (Windows) or the ChemDraw Folder (Macintosh)).

ChemDraw (*.cdx)

The ChemDraw file format is the native format for ChemDraw version 4.0. This is a public tagged file format that stores information about a ChemDraw structure in a series of data blocks. This format is designed to be easily generated and interpreted by other programs. This format accurately stores anything that can be drawn in ChemDraw.

NOTE: Imported pictures saved within a ChemDraw version 4.0 file created using ChemDraw for Macintosh will be lost when the file is opened using ChemDraw for Windows. However, all ChemDraw specific information is preserved. Imported pictures include any graphics pasted into a ChemDraw document from another Macintosh application. The same applies for Windows to Macintosh conversion.

ChemDraw 3.5 (*.chm)

ChemDraw 3.5 file format are used for saving or opening ChemDraw documents using the version 3.5.x of ChemDraw. These documents can also be opened in versions 3.0, 3.0.1, 3.0.2, and 3.1 of ChemDraw as long as atom properties are not used in the files.

NOTE: When you save a ChemDraw version 4.0 file in one of these formats, all features specific to version 4.0 are lost. For instance, multi-attached atom labels, variable attachment points, and multicenter bonds will not be saved.

ChemDraw 2.0 and ChemDraw 2.1 (*.chm)

ChemDraw 2.0 and ChemDraw 2.1 file formats are used for saving or opening ChemDraw documents using the version 2.x file format of ChemDraw for Macintosh.

NOTE: When you save a ChemDraw version 4.0 file in one of these formats, all features specific to version 4.0 are lost. For instance, color, dative bonds and shaded orbitals will not be saved.

ChemDraw Stationery/Style Sheet (*.cds)

ChemDraw Stationery file format is used for saving document settings and other objects. See the section titled "Saving Customized Settings" in Chapter 1, *ChemDraw Basics*, for more information.

Connection Table (*.ct)

The Connection Table file format is a simple format that saves a list of atom connectivities in terms of an element, serial number, X and Y coordinates, bond order and bond type. This is a common format used for exchanging information between many chemistry applications.

[PRO] DARC-F1 Format *.f1d (Export only)

The native file format for storing structures in the Questel DARC system.

[PRO] DARC-F1 Query *.f1q (Export only)

The native file format for storing queries in the Questel DARC system.

Encapsulated PostScript (Text) (Macintosh) PostScript, *.eps (Windows) (both Export only)

Encapsulated PostScript (Text) files, also referred to as EPS (Text), are ASCII text files containing the scalable PostScript representation of a ChemDraw picture that can be opened using other platforms and applications and platforms. No preview is included in this type of EPS file. Thus, programs that do not support the display of raw PostScript can only print, not view an image on screen.

EPS files are commonly used for sharing ChemDraw pictures with desktop publishing applications such as Adobe PageMaker and QuarkXPress.

All colors are saved in the EPS file except for the Background color.

NOTE: To save an EPS file with a colored background, create a large colored rectangle and choose Send to Back before saving the file.

Encapsulated PostScript (Macintosh)

Encapsulated PostScript (Macintosh) files, also referred to as EPS (Mac) files, contain both the scaleable PostScript representation and the QuickDraw representation of a ChemDraw picture that other Macintosh applications can translate and view. ChemDraw pictures saved in EPS (Mac) file format can be opened by various illustration, desktop publishing and desktop presentation software packages on the Macintosh.

EPS (Mac) files created by earlier versions of ChemDraw can be opened by ChemDraw version 4.0.

All colors are saved in the EPS file except for the Background color.

NOTE: To save an EPS file with a colored background, create a large colored rectangle and choose Send to Back before saving the file.

GIF Image *.gif (Export only)

You can save your ChemDraw document in the graphics interface format, GIF. This file format is useful for working with the hypertext markup language (HTML) used in displaying information on the World Wide Web. A GIF image can be displayed directly on a Web page rather than having to download the picture for viewing in a Helper application.

ChemDraw always saves GIF files according to the 89a specifications with transparent backgrounds.

PRO ISIS/SKC and ISIS/TGF

In addition to Clipboard compatibility, you can also save a ChemDraw document in an ISIS file format for export to an ISIS application, or import a file created by an ISIS application into ChemDraw. ChemDraw Pro provides two File format:

ISIS/Sketch (*.skc) for saving files as a binary sketch file for transfer to another ISIS application running under Windows or Macintosh (this is the format used on the Clipboard as well); ISIS/TGF (*.tgf) for saving as an ASCII text file (a Transportable Graphics File) for transfer to ISIS applications on other platforms.

NOTE: When transferring between ChemDraw and ISIS/Draw, if information in a file or on the Clipboard contains only non-bond, unsupported objects, the information is imported as a WMF (metafile) or PICT graphic. However, if a supported object, such as a bond, is also in the file or on the Clipboard, then only the supported object appears.

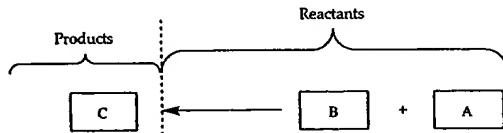
NOTE: Object types in ISIS not supported in ChemDraw, such as polygons, are not transferred. Object types in ChemDraw not supported in ISIS are not transferred. However, in some cases, such as different arrow types, the arrow is converted to the most similar form. If text in an ISIS Superatom matches a Nickname in ChemDraw it is represented in ChemDraw using the Nickname. If the text does not match a Nickname you are alerted and asked to either copy the Superatom as a label without any chemical significance, or to expand the Superatom and paste it as a structure. See "Nicknames" in Chapter 8, Advanced Drawing Techniques.

PRO ISIS/Reactions (*.rxn)

The ISIS/Reactions format, also referred to as RXN is an MDL-developed format for storing chemical reaction information, used by the ISIS family of products among others.

NOTE: To determine which molecules in a reaction are reactants and which are products, ChemDraw uses the point of the reaction arrow as the dividing line. Molecules whose centers are behind the tip of the arrow are considered reactants, and all remaining molecules are products. The reaction arrow can be at any orientation, i.e., it does not have to be parallel to the x-axis. If a reaction contains multiple arrows, then the largest arrow is used as the reaction arrow.

Figure 13-13 A reaction scheme



NOTE: ChemDraw will only recognize structures. Symbols, such as "+", will be ignored.

PRO MDL MolFile (*.mol)

Molecular Design Limited MolFile (MDL MolFile) file format is used by several other Windows, Macintosh and UNIX chemical databases and drawing applications such as ISIS/Draw™, ISIS/Base™, MACCS™, and REACCS™. There are two MDL MolFile formats provided in ChemDraw Pro: MDL MolFile (Text) and MDL MolFile (Mac). MDL MolFile files are ASCII text files that can be created or edited in common word processing applications or text editors.

PRO Molecular Simulations MolFile (*.msm)

Molecular Simulations MolFile format is an ASCII text file used by applications such as ChemNote™. You can save a ChemDraw Pro document in Molecular Simulations MolFile format for export to one of these applications.

NOTE: ChemDraw version 4.0 uses the file extension ".msm" for Molecular Simulations MolFiles rather than the standard ".mol", used by Molecular Simulation, Inc. ChemDraw recognizes files with the ".mol" file extension as MDL MolFiles. In addition, the extension ".msi" used in earlier versions of ChemDraw is no longer recognized in ChemDraw 4.0. To open Molecular Simulations MolFiles that have a ".mol" or ".msi" extension you must first change the extension to ".msm".

PICT (Macintosh)

PICT files contain a QuickDraw representation of a ChemDraw picture that can be used by various drawing applications. You can save a ChemDraw document in the PICT format so it can be opened by one of these other applications. The PICT file format contains ChemDraw structural information. PICT files created by ChemDraw version 4.0 or earlier can be reopened and edited by ChemDraw version 4.0. PICT files created by ChemDraw 4.0 can be edited by ChemDraw 3.x, but not by earlier versions of ChemDraw.

All colors are saved in the PICT file except for the Background color.

PICT scaled 4X (Macintosh)

PICT scaled 4x files are the same as PICT files, except that the drawing is four times larger. When these larger files are placed into certain other applications and shrunk back down to $\frac{1}{4}$ size, they may provide higher quality output than regular PICT files.

PRO SMD

Standard Molecular Data (SMD) file format, version 4.3, is an ASCII text file commonly used by programs that search Chemical Abstracts Databases such as STN Express™. You can save your ChemDraw document in SMD format and use the file for searching in a Chemical Abstracts database.

Template Style Sheet (*.cts)

The Template Style Sheet file format is used for saving document settings and row and column characteristics for creating *ChemDraw* Template documents.

Windows Metafile (Windows Only) (*.wmf)

The Windows Metafile file format saves the GDI representation of a *ChemDraw* picture. Using the WMF file format you can transfer *ChemDraw* pictures to other applications, such as *Word* for Window, that support that WMF file format on the same or different computers rather than using the Clipboard. The WMF file format contains *ChemDraw* structural information. WMF files created by *ChemDraw* version 4.0 or earlier can be reopened and edited by *ChemDraw* version 4.0. WMF files created by *ChemDraw* 4.0 can be edited by *ChemDraw* 3.x.

Appendix A, The Chemistry of ChemDraw

As you work, *ChemDraw* automatically converts your various lines, characters, and other symbols into chemically meaningful figures. Normally, much of this work is silent, but you can choose to view this chemical data using the Check Structure, Analyze Structure, and Expand Atom Labels commands. *ChemDraw* also uses this chemical data when exporting to file formats that support only a subset of the notations that *ChemDraw* does.

This appendix illustrates how *ChemDraw* uses its chemical intelligence to interpret what you have drawn. It also shows some of the ways you can help *ChemDraw* better understand what you mean. Also discussed are a few cases where *ChemDraw* might not understand what you think is a perfectly reasonable diagram.

IS ALL OF THIS REALLY NECESSARY?

In a word, *no*. *ChemDraw* was designed as a tool to aid in chemical communication, but it is a tool only. Walk up to any chemist and say "benzene," and both of you will immediately understand what substance is being discussed. Similarly will you be understood if you draw a six-membered ring of alternating single and double bonds, regardless of the size, color, orientation, or thickness of the ring itself — and regardless of what *ChemDraw* thinks about it.

Still, just because it is not necessary does not mean it is not useful. If you're investigating organic acids, a compound with the structural formula CH₃COO would most probably represent acetic acid; present the same formula in a paper on transition metal chemistry, and you might be describing a novel methylated cobalt oxide. If you had asked *ChemDraw* what it thought beforehand, you would have received a message reporting a valence error, and you might have been prompted either to add a negative charge or to change the capitalization.

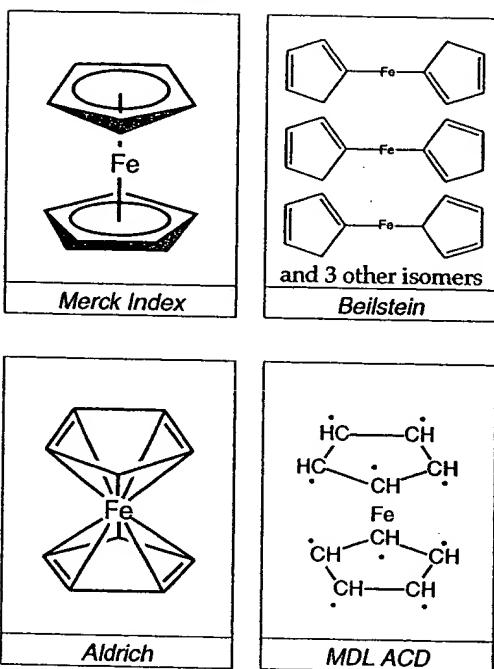
In this way *ChemDraw*'s chemical intelligence can be used as a sophisticated "spelling" checker for chemical compounds.

It is important to remember that chemists are generally a whole lot smarter than computers. Most chemists would understand AcOo-C₆H₄COOH immediately, whether or not they recognized it as aspirin. Most computer programs, however, require what is known as a "complete connection table," in this case a collection of 21 atoms connected by 5 double bonds and 16 single bonds in a specific pattern. With its chemical intelligence, *ChemDraw* can take what makes sense to you as a chemist, and convert it into what makes sense to another application.

There are conventions, and there are conventions...

Unfortunately, making sense is only half the battle when searching chemical databases. Most databases require not only that you draw a structure in a way that makes sense, but that you draw it in *the* way that they expect. Consider ferrocene, which is represented in at least four different ways in major databases:

Figure A-1 Ferrocene



A successful search in one database might produce absolutely no hits in another. When in doubt, consult the documentation for your database, and see if it offers any clues to the conventions used.

But that's not what I mean!

ChemDraw can offer only suggestions, and when it comes down to it, *ChemDraw*'s suggestions don't matter. If you and your audience both understand what you are trying to depict, then you should rightly ignore *ChemDraw*'s complaints. In many cases you can silence *ChemDraw* permanently by teaching it to understand the notation you're using. For more information, see "Nicknames" in *Chapter 8, Advanced Drawing Techniques*.

CHEMISTRY IN CHEMDRAW

The remainder of this chapter focuses on the chemical conventions understood by *ChemDraw*.

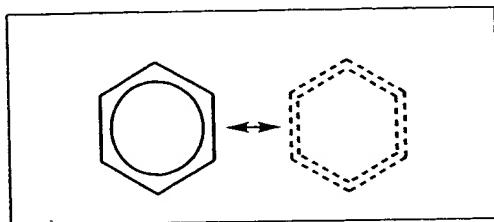
Bonds

Table A-1 Types of bonds

- Single bond, unspecified stereochemistry.
- - - Single bond, "down" stereochemistry (into the plane of the paper, away from the viewer), *from* the first drawn atom *to* the second drawn atom.
- — — Single bond, "up" stereochemistry (out of the plane of the paper, toward the viewer), *from* the first drawn atom *to* the second drawn atom.
- ~~~~ Single bond, mixture of "up" and "down" stereochemistries in some unspecified proportion.
- Dative bond. Often used to indicate polar bonds in N-oxides, for example.
- == Double bond, with *cis / trans* stereochemistry as drawn.
- × Double bond, with *cis / trans* stereochemistry unknown.
- Tautomeric bond, either single or double according to rules of tautomerism.
- ===== Aromatic bond, part of a delocalized resonance system.
- ==== Triple bond.

In addition, a single bond near a closed circle will be recognized as aromatic:

Figure A-2



Atom Labels

A simple atom label may contain any of the following:

Table A-2 Types of atom labels

<chem>—Cl</chem>	A single element.
<chem>—O</chem>	
<chem>—CH3</chem>	An element and some number of hydrogens.
<chem>—N</chem>	
<chem>—Me</chem>	A nickname.
<chem>—Ala</chem>	
<chem>—C(OCH3)3</chem>	Repeating units within parentheses.
<chem>—O(CH2)4CH3</chem>	
<chem>—CH2COOC(OPh)3</chem>	A series of any combination of the above.

When analyzing an atom label, *ChemDraw* generally starts at the left and continues to the right, applying standard rules of valence to determine which atoms are bound to which. The exception is with an atom label in Automatic alignment on the left side of a compound. This sort of atom label is displayed "backwards" (H3CO instead OCH3) and is therefore parsed from right to left. Standard valences for each atom are defined in the Isotopes Table (Macintosh) or isotopes.txt (Windows).

By definition, a "simple" atom label has all bonds attached to the first (or last) character. A multi-attached atom label has bonds connected to more than one character, or has all of its bonds attached to a specific character in the middle of the atom label. Multi-attached atom labels are always parsed from beginning to end, but again the beginning might be on the right if the atom label was in Automatic style and on the left side of the original structure:

Table A-3 Types of multi-attached atom labels

<chem>—O</chem>	A multi-attached label that is parsed from left to right.
<chem>—CH2C(=O)CH3</chem>	
<chem>—O</chem>	A multi-attached label that is parsed from right to left.
<chem>—(CH2)4OH</chem> ↓ <chem>—CH2(CH2)3OH</chem>	A bond attached to the open parenthesis of a repeating group is treated as if bonded to the first of those groups.
<chem>—(CH2)4</chem> ↓ <chem>—CH2(CH2)2CH2</chem>	A bond attached to the close parenthesis or repeat count of a repeating group is treated as if bonded to the last of those groups.

Chemically-significant Text

Often it is simpler to write a chemical formula like MeOH or H₂O than it is to draw out an entire atoms-and-bonds structure. *ChemDraw* will correctly interpret any *unambiguous* structural formula. In this way, CH₃COCH₂CH₃ is recognized as methyl ethyl ketone; MeOH is recognized as methanol. On the other hand, C₆H₆ might mean benzene, or it might mean one of over 200 other isomers. C₆H₆ is not recognized by *ChemDraw*, and will generate an error message if you try to analyze it. Generally, empirical formulas (C₂H₆ and H₂SO₄) are not recognized, but structural formulas (CH₃CH₃ and HOSO₂OH) are.

Chemically-significant text must be entirely in Formula or (for isotopes and charges) Superscript style. *ChemDraw* will not recognize a chemical formula embedded within a larger block of text.

Table A-4 Examples of chemically-significant text

NH ₄ ⁺	If you draw a bond, add an atom label, then delete the bond, you have a chemically meaningful text block whose font, size, and style match other atom labels.
H ₂ O	If you create a caption with the text tool and set it to Formula style, you have a chemically meaningful text block whose font, size, and style match other captions.

Charges

Charges may be created as part of a textual atom label or with the appropriate symbol from the Chemical Symbols Palette. Charges are always assigned to a specific element in the atom label, whose acceptable valences become those of the similar isoelectronic neutral element.

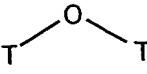
Table A-5 Examples of charges

—O-	A charge following an element is assigned to that element.
—+NH ₃ ↓ —(N+)H ₃	A charge that does not follow an element is assigned to the next element.
—NH ₃ ⁺ ↓ —(N+)H ₃	Charges that follow a monovalent element with a repeat count are assigned to the element before that element.
—CO ₂ ↓ —CO(O ⁻)	Charges that follow other repeating units are distributed among those units.
—NH ₃ ⁺	Charges may be superscripted.
—Fe ⁺⁺	Multiple charges are recognized appropriately.
—Fe ²⁺	Charges may have repeat counts as long as both the charge and the repeat count are superscripted.
⊕ —NH ₃ ↓ —(N+)H ₃	A “floating” charge placed with the Chemical Symbols Tool is assigned to the nearest atom. (If no atom is within the distance set as the Fixed Length, the charge is ignored and not assigned to any atom).

Isotopes

By default, *ChemDraw* will correctly recognize all isotopes in the full Table of the Elements; this data has been provided by CRC Press, Inc². Isotopes are defined in the Isotopes Table (Macintosh) or isotopes.txt (Windows). In the extremely unlikely event that you need to modify add new isotopes, this file can be edited with any text editor.

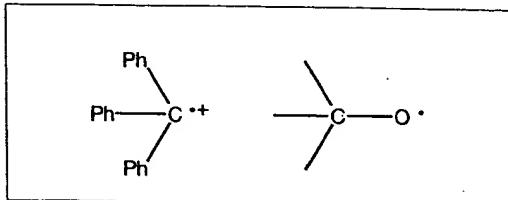
Table A-6 Examples of isotopes

$\text{---}^{35}\text{Cl}$	Isotope numbers are indicated by a super-scripted number before the element symbol.
$\text{---CH}_2^{13}\text{COOH}$	Isotopes can be included anywhere that regular elements can.
	Deuterium and Tritium can be indicated by their one-letter symbols.
$\text{D}_3\text{C---OD}$	

Radicals

Radicals are indicated with the appropriate symbol from the Chemical Symbols Palette. As with charges, they are assigned to the nearest atom. Radicals always occupy one free valence, in addition to any charge effects.

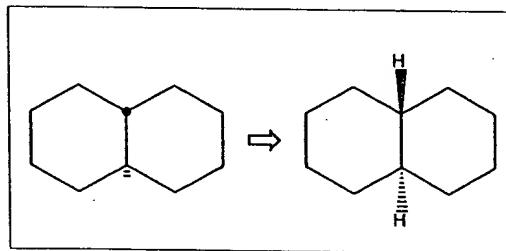
Figure A-3 Examples of radicals



H-Dot/H-Dash

H-Dot and H-Dash symbols from the Chemical Symbols Palette indicate the stereochemistry of a single hydrogen atom. These symbols are most commonly used in fused systems.

Figure A-4 Examples of H-Dot/H-Dash



Complexes

Compounds with electron pairs can act as Lewis bases, bonding with Lewis acids that are electron-deficient. Similar behavior can be seen between lone pairs and metals.

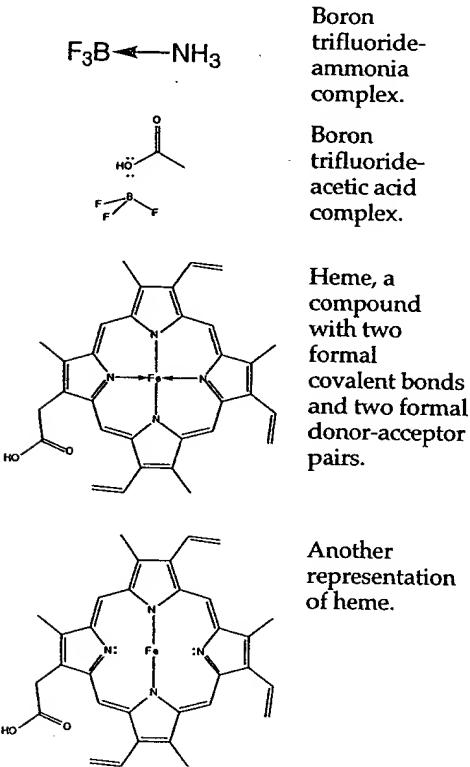
The best representation of these types of interaction is with a dative bond *from* the electron-pair donor *to* the acceptor. With a plain bond instead of the dative one, *ChemDraw* would report a valence error. The dative bond more accurately represents the electron donation.

Complexes may also be represented with explicit lone pairs and without any bonds at all.

² Adapted from the *Table of Isotopes* data, in the CRC Handbook of Chemistry and Physics, 77th Ed., Lide, D.R., Editor-in-Chief, CRC Press, Boca Raton, Florida, ©1996. With permission.

If you do use a plain bond to indicate a complex, you may wish to set Abnormal Valence to Allowed in the Atom Properties dialog.

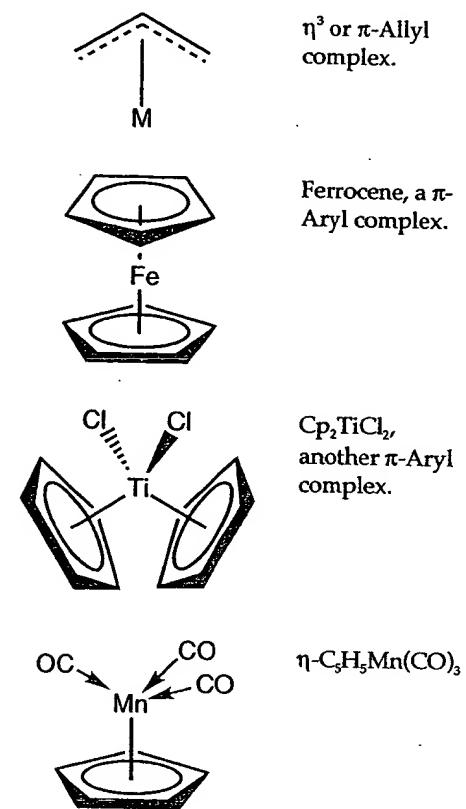
Table A-7 Examples of complexes



Multi-center Attachments

Multi-center attachments are meaningful only when created using the Add Multi-Center Attachment command from the File Menu. This command creates a pseudo-atom that is disregarded during chemical calculations, but still allows you to create diagrams that look meaningful to the experienced chemist.

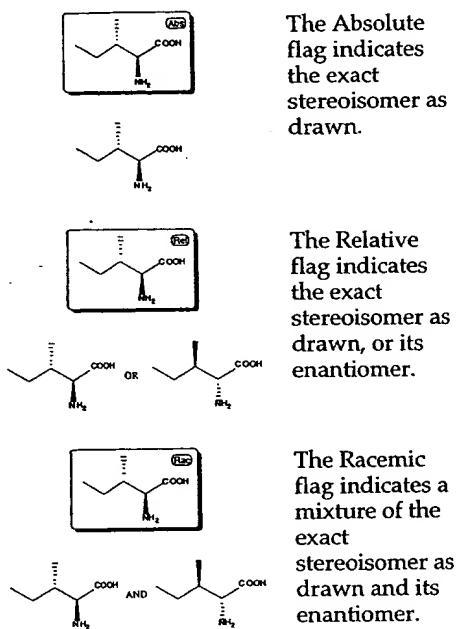
Table A-8 Examples of multi-center attachments



Stereochemical Flags

While the chirality of a specific stereocenter can be indicated with the appropriate wedged, hashed, or plain bond, sometimes it is useful to indicate the relative stereochemistry of a molecule as a whole, considering the relationship between all stereocenters. Stereochemical flags apply to the nearest structure; if no structure is within the distance specified by the Fixed Length value, the stereochemical flag is not assigned to any structure.

Table A-9 Examples of stereochemical flags



Query Properties

By their nature, query properties do not represent actual chemical features, but rather describe broad classes or groups of features. For information on using query properties, see *Chapter 9, Drawing Query Structures*.

Analysis Messages

Occasionally, *ChemDraw* may be unable to analyze your structure fully for one reason or another. There are two general types of messages: status messages that report a problem that might not affect the final analysis, and critical messages that probably will.

Table A-10 Examples of analysis messages

There are too many bonds to this unlabeled Carbon.	Displayed for every unlabeled atom with more than 4 filled valences. Filled valences include sum of bond orders, charge, radicals, and free sites. Aromatic bonds count 1.5 each, rounded down unless it is the only bond to the atom. Charge is signed and includes charge implied by dative bonds. The Substituents query property treats Free Sites, Up to and Exactly the same way, that is, an atom with 2 explicit bonds and "Substituents: Up To 3" or "Substituents: Exactly 3" or "Substituents: Free Sites 1" has three filled valences.
An atom in this label has an invalid valence.	Displayed in a variety of cases where <i>ChemDraw</i> cannot find a place to put a bond or cannot find a bond to put on an atom. Valid valences for each element are listed in the Isotopes Table (Macintosh) or isotopes.txt (Windows).
ChemDraw can't interpret this label.	Displayed when <i>ChemDraw</i> finds text that it cannot identify as an element, nickname, generic nickname, or alternative group name.
Parentheses don't match.	Displayed when parentheses cannot be matched into nested open-close pairs.
This label has conflicting or unassignable charges.	Displayed when a plus and minus charge have been assigned to the same element, charges have been assigned in more than one way, or a charge has been assigned to a nickname, generic nickname, or Alternative Group name.

**Table A10 Examples of analysis messages
(continued)**

An unknown error occurred in the label interpreter.	You should never see this message. If you do, please contact CambridgeSoft Technical Support with information on the label that produced it. See <i>Appendix C, Technical Support</i> , for more information.	This named alternative group contains fragments with inconsistent valences.	Displayed for any Alternative Group Box whose contained structures have varying numbers of attachment points. Since all structures within an Alternative Group Box are to be used interchangeably, they must have the same number of attachments. This is a status message only.
Odd-membered heteroaromatic rings must be drawn with explicit double bonds.	Displayed for every circle in an odd-sized ring. This is a status message only; analysis will continue but may produce inaccurate results.	This named alternative group contains no fragment.	Displayed for any Alternative Group Box that is empty. This is a status message only.
Formula cannot be computed for queries.	Displayed for every label that contains a generic nickname, an element list or an alternative group. This is a status message only; analysis will continue as if the problematic label were not selected.	Part of a molecule is outside of the alternative group definition.	Displayed for any Alternative Group Box whose border crosses part of a structure. This is a status message only.
Text not in Formula style won't be interpreted.	Displayed for the first caption that is not an atom label or Alternative Group name, and which contains any text not in Formula, Subscript, or Superscript style. This is a status message only, and will appear only once regardless of how many captions are in the selection.		
This named alternative group contains no attachment point.	Displayed for any structure within an Alternative Group Box where the structure lacks an attachment point. This is a status message only.		

Appendix B, Specifying Paths

This appendix describes the path information necessary to locate the cd_items directory under Windows or the ChemDraw Folder on the Macintosh.

WINDOWS

Normally, the cd_items directory is in the same directory as the *ChemDraw* application and the path is automatically set. However, if you want the cd_items folder to reside in a different directory, you must specify the path in the chemdraw.ini file.

When the path is not specified properly, *ChemDraw* displays an error message and quits.

To change the path in the chemdraw.ini file if you are using Windows:

- Open the chemdraw.ini file using a text editor, such as the Windows Notepad application found in the Accessories program group.

NOTE: You should always create a backup of the chemdraw.ini file before you make any edits. Use the backup file if for any reason the edited file does not work properly.

Normally, the chemdraw.ini file is located within your Windows directory.

The following is an example of the text that appears:

```
cd_items_PATH=C:\CHEMDRAW\cd_items  
WindowPosition=10, 10, 712, 561  
PalettePostion=14,52
```

The path information for the cd_items directory is specified in the line beginning with "cd_items_PATH=". If this line doesn't exist, you should create it, otherwise *ChemDraw* looks for the cd_items directory in your local directory.

To specify the path (Information within the chemdraw.ini file isn't case sensitive):

- Type the path after "cd_items_PATH="

For example, if the cd_items directory is located within a directory called "users" on drive C, type:

- c:\users\cd_items

The complete line would read
"cd_items_PATH=c:\users\cd_items"

After specifying the path:

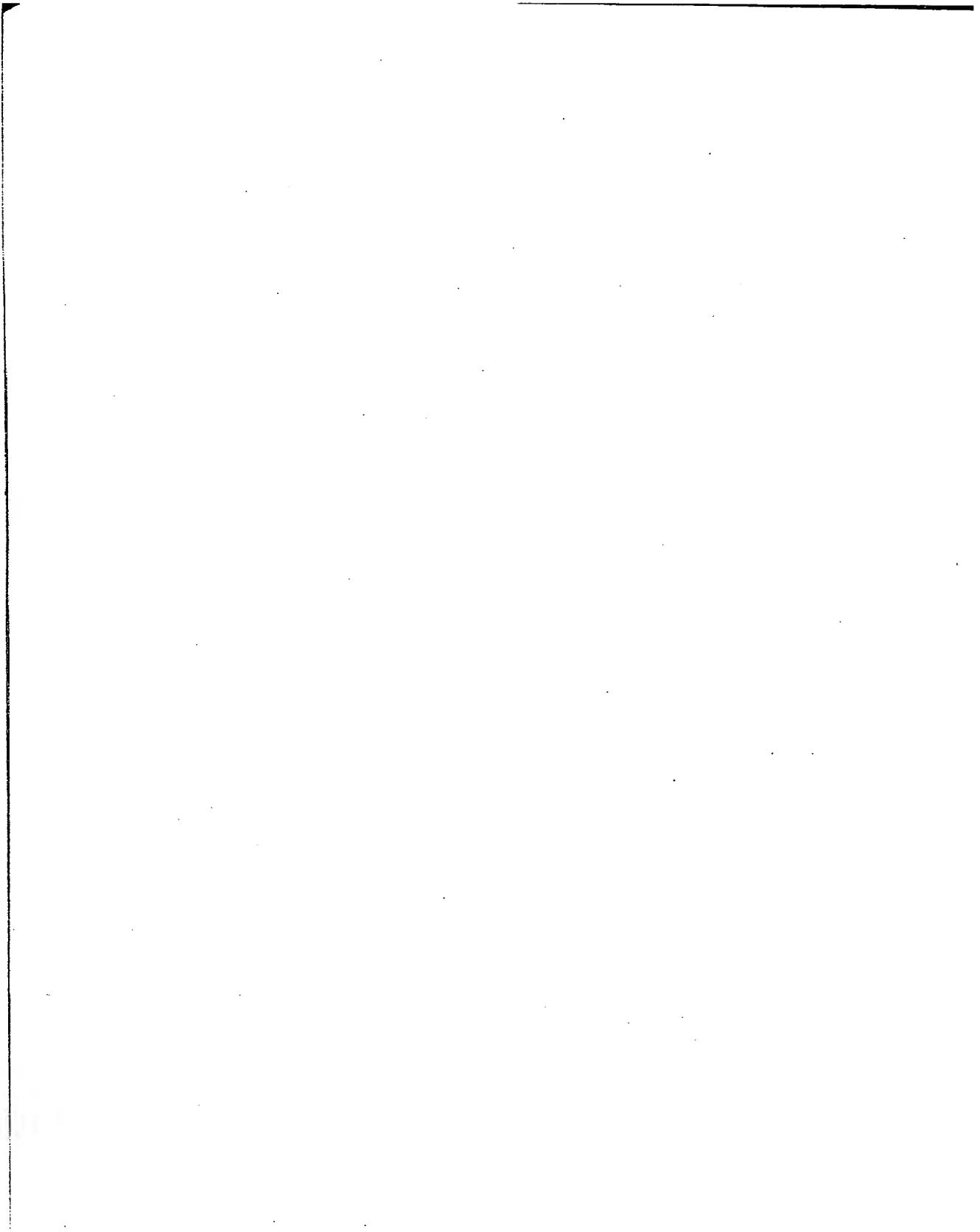
- Save the changes and close the chemdraw.ini file.

To implement the changes:

- Exit and restart *ChemDraw*.

MACINTOSH

When ChemDraw 4.0 is installed the ChemDraw Folder is placed in the same folder as the application. However, if you are using ChemDraw from a file server and you want to have your own ChemDraw folder, place the ChemDraw folder in the Preferences folder in your System folder. ChemDraw will always look for the ChemDraw folder in the Preferences folder first, followed by the application folder second.



Appendix C, Technical Support

CambridgeSoft Corporation (CS) provides technical support to all registered users of this software through the World Wide Web (WWW), and through our Technical Support department.

Our Technical Support pages on the WWW contain answers to frequently asked questions (FAQs), in addition to some general information about our software. You can access our Technical Support page using the following address:

<http://www.camsoft.com/support/>

If you don't find the answers you need on the WWW, please complete the following tasks before contacting the Customer Support Department.

Step 1: Check the Readme file for known limitations or conflicts.

Step 2: Check the system requirements for the software at the beginning of this user's guide.

Step 3: Read the Troubleshooting section of this appendix and follow the possible resolution tactics outlined there.

Step 4: If all your attempts to resolve a problem fail, fill out a copy of the CS Software Problem Report Form at the back of this user's guide. This form is also available on-line through our WWW Technical Support page.

- Try to reproduce the problem before contacting us. If you can reproduce the problem, please record the exact steps that you took to do so.
- Record the exact wording of any error messages that appear.
- Finally, please record anything that you have tried to correct the problem.

You can deliver your CS Software Problem Report Form to Technical Support by the following methods:

Internet: support@camsoft.com

CompuServe: 76070,615

America On-line: CamSoft

Fax: 617 491-7203

Mail:

CambridgeSoft Corporation
ATTN: Technical Support
875 Massachusetts Avenue
Cambridge, MA 02139 USA

SERIAL NUMBERS

When contacting Technical Support, you must *always* provide your serial number. This serial number was on the outside of the original *ChemDraw* box, and is the number that you entered when you launched *ChemDraw* for the first time. If you have thrown away your box and lost your installation instructions, you can find the serial number in the following ways:

Macintosh

- With *ChemDraw* launched, choose About CS *ChemDraw* from the Apple menu. The serial number will appear at the bottom left of the about box.
- In the Finder, single-click on the *ChemDraw* application icon and choose Get Info from the File menu. The serial number will be listed immediately after the version.

Windows

- With *ChemDraw* launched, choose About CS *ChemDraw* from the Help menu. The serial number will appear at the bottom left of the about box.
- Open the chemdraw.ini file (in your Windows directory) using any text editor. The serial number will appear in the line starting "SERIAL_NO=".

TROUBLESHOOTING

This section describes steps you can take that affect the overall performance of *ChemDraw*, as well as steps to follow if your computer crashes when using a CS software product.

Launching

If *ChemDraw* can't find the *ChemDraw* Folder (Macintosh) or *cd_items* directory (Windows) you will not be able to launch the program. See Appendix B, Specifying Paths for additional information about the appropriate location.

Performance

Below are some ways you can optimize the performance of *ChemDraw*:

Step 1. Installing the non Power Macintosh version of a CS product on a Power Macintosh will likely decrease performance.

Step 2 (Macintosh): Increase the total amount of memory that the application can use:

- Select the *ChemDraw* application icon in the Finder when *ChemDraw* is not running.
- From the Edit menu, choose Get Info. Increase the memory allocation in the Preferred size text box in the Memory Requirements section of the dialog box.

Step 2 (Windows) In the "386 Enhanced" control panel (Windows 3.1, 3.1.1, and Windows for Workgroups), the "System" control panel (Windows NT 3.5.1) or the "Performance" tab in the System control panel (Windows 95 or Windows NT 4.0), allocate more processor time to *ChemDraw*.

Step 3: Install more physical RAM. The more you have, the less *ChemDraw* will have to access your hard disk to use Virtual Memory.

Step 4 Increase the Virtual Memory (VM). Virtual memory extends RAM by allowing space on your hard disk to be used as RAM. However, the time for swapping between the application and the hard disk is slower than swapping with physical RAM. Here is where you can change VM:

- **Macintosh:** Memory control panel.

NOTE: If you are running a Power Macintosh, the optimum virtual memory setting is one MB greater than the physical RAM. Any changes – either by increasing the virtual memory or by turning it off altogether – will significantly lower performance.

- **Windows 3.1:** 386 Enhanced control panel.
- **Windows 95 and Windows NT 4.0:** Performance control panel.
- **Windows NT 3.5.1:** System control panel.

System Crashes

ChemDraw should never crash, but below are the steps you should go through to try to resolve issues that cause computer crashes while using a CS software product.

Step 1: Restart your computer (Macintosh), or restart Windows. Next, try to reproduce the problem. If the problem does reoccur, keep reading.

Step 2 (Macintosh): Restart your computer while holding the Shift key down to turn off all system extensions. Try to repeat the problem.

If the problem no longer occurs, then you likely have an extension conflict. You should determine which extension is causing the conflict, and then not have it load when using *ChemDraw*. To isolate an extension, disable half of your extensions using the Extension manager and test the problem again. Keep disabling half of your extensions until you find which extension(s) are causing the problem. Please inform Technical support which extension(s) is/are causing the problem.

Step 2 (Windows): The most common conflicts for Windows users concern Video Drivers, Printer Drivers and Win32s conflicts (if you are running under Windows 3.1, 3.11 or Windows for Workgroups). If you do end up needing to contact us, be sure to determine what type of drivers you are using and the version of Win32s if you are using Windows 3.1.

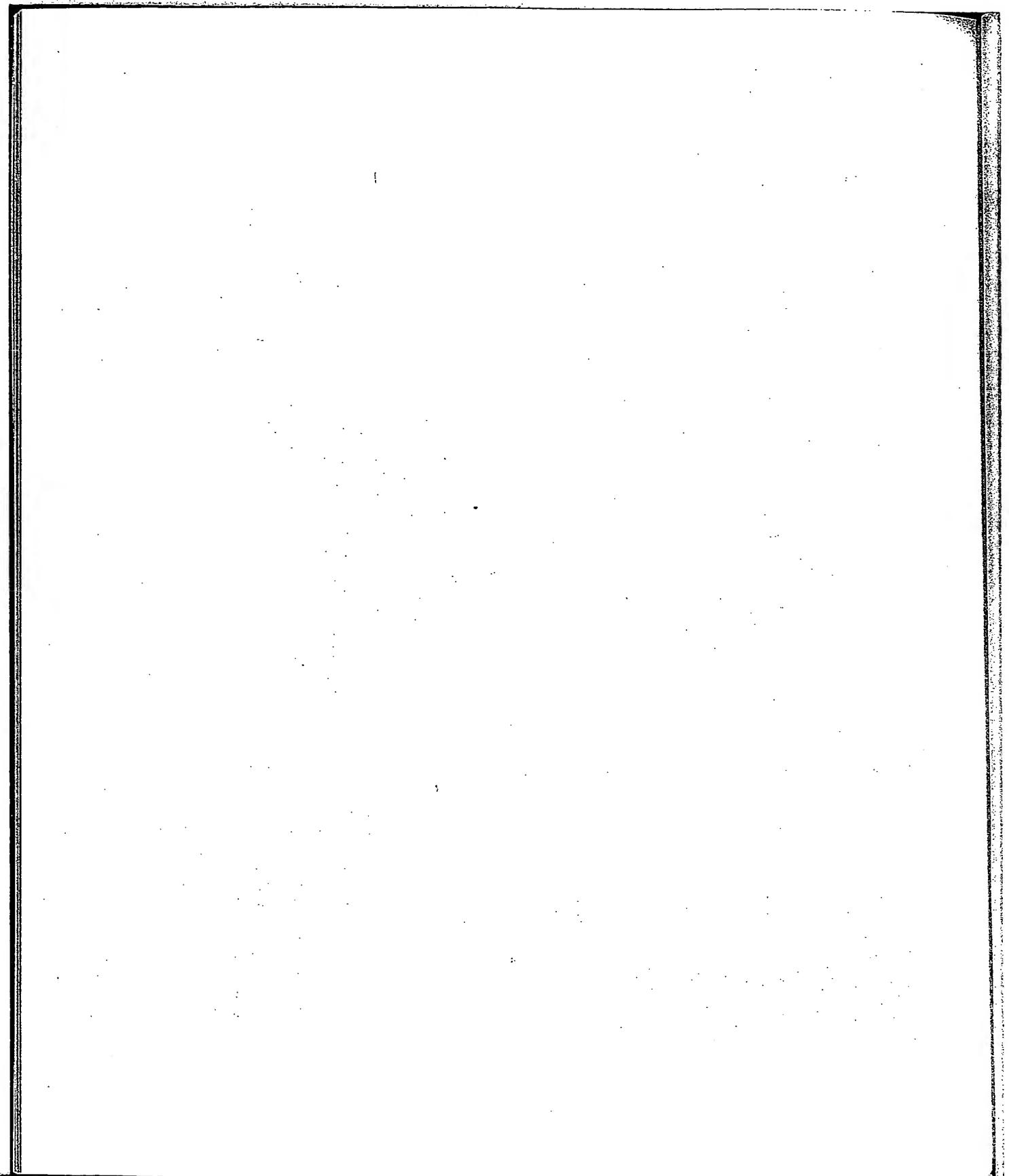
Video Driver related problems: If you are having problems with the display of ChemDraw, try switching to the VGA video driver in the display Control Panel (or System Setup then retest the problems. If using a different driver helps, your original driver may need to be updated--contact the maker of the driver and obtain the most up-to-date driver. If you still have trouble contact us with the relevant details about the original driver and the resulting problem.

Printer Driver related problems: Try using a different printer driver. If using a different driver helps, your original driver may need to be updated--contact the maker of the driver and obtain the most up-to-date driver. If you still have trouble contact us with the relevant details about the original driver and the resulting problem.

Win32s related problems: For Windows 3.1, 3.11 and Windows for Workgroups users, make sure you have the latest version of Win32s. This can be downloaded from Microsoft's WWW or FTP sites.

Step 3 (All): Try reinstalling the software. For users of Windows 3.1, Windows 3.11 or Windows for Workgroups you must uninstall the software before reinstalling. See the complete uninstall instructions on the Technical Support page on the WWW.

Step 4: If it still occurs, Fax or Email the details of the problem to customer support.



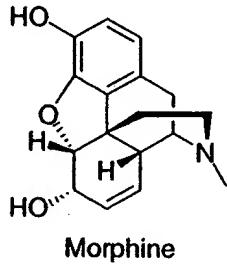
Appendix D, Document Settings

This Appendix contains a table of drawing setting and an example structure for each of the style sheets/stationery pads shipped with *ChemDraw*.

NOTE: Creating your own style sheets/stationery pads is easy. Simply create a new document, enter the settings in the Page Setup, Drawing, Text Settings and Color Palette dialog box and choose Save Stationery/Style Sheet from the File menu. In the dialog box, make sure the ChemDraw Style Sheet (Windows) or ChemDraw Stationery (Macintosh) file format is selected, type a name for the document, choose the location for saving as cd_items directory (Windows) or ChemDraw Folder (Macintosh) and click the OK button (Windows) or Save button (Macintosh).

Table D-1 Drawing and Text (atom label and caption) Settings in Journal Style Sheets/Stationery Pads

ACS-1996

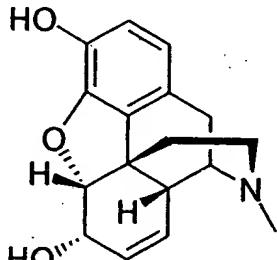


Morphine

Fixed Length: 14.4 pt
Bold Width: 2 pt
Line Width: 0.6 pt
Margin Width: 1.6 pt
Hash Spacing: 2.5 pt
Chain Angle (degrees): 120
Bond Width (% of length): 18
Atom Label Font (Win/Mac): Arial / Helvetica
Atom Label Size: 10 pt
Caption Font (Win/Mac): Arial / Helvetica
Caption Size: 10 pt
Drawing Area (Width x Height): 540 pt x 720 pt
Page Size: US Letter
Reduction (%): 100

Table D-1 Drawing and Text (atom label and caption) Settings in Journal Style Sheets/Stationery Pads
(continued)

Can. J. Chem.



Morphine

Fixed Length: 18 pt

Bold Width: 2.5 pt

Line Width: 0.8 pt

Margin Width: 2 pt

Hash Spacing: 3 pt

Chain Angle (degrees): 120

Bond Width (% of length): 18

Atom Label Font (Win/Mac): Arial/Helvetica

Atom Label Size: 12 pt

Caption Font (Win/Mac): Arial/Helvetica

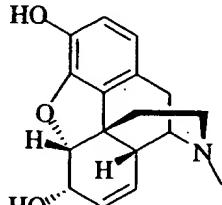
Caption Size: 12 pt

Drawing Area (Width x Height): 540 pt x 720 pt

Page Size: US Letter

Reduction (%): 80

J. Mol. Mod.



Morphine

Fixed Length: 14.4 pt

Bold Width: 2 pt

Line Width: 0.6 pt

Margin Width: 1.6 pt

Hash Spacing: 2.5 pt

Chain Angle (degrees): 120

Bond Width (% of length): 18

Atom Label Font (Win/Mac): Times New Roman/Times

Atom Label Size: 10 pt

Caption Font (Win/Mac): Times New Roman/Times

Caption Size: 10 pt

Drawing Area (Width x Height): 8.5 cm x 25.4 cm (1 column)

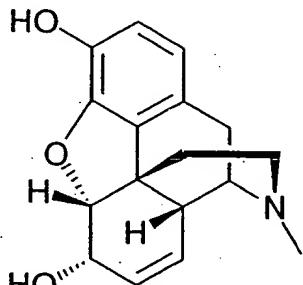
17 cm x 25.4 cm (2 column)

Page Size: US Letter

Reduction (%): 100

Table D-1 Drawing and Text (atom label and caption) Settings in Journal Style Sheets/Stationery Pads
(continued)

RSC-1995



Morphine

Fixed Length: 0.7 cm

Bold Width: 0.092 cm

Line Width: 0.025 cm

Margin Width: 0.071 cm

Hash Spacing: 0.099 cm

Chain Angle (degrees): 120

Bond Width (% of length): 20

Atom Label Font (Win/Mac): Arial/Helvetica

Atom Label Size: 12 pt

Caption Font (Win/Mac): Arial/Helvetica

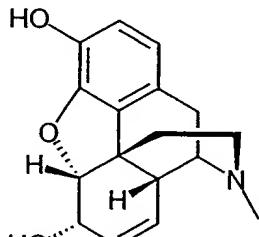
Caption Size: 12 pt

Drawing Area (Width x Height): 19.05 cm x 25.4 cm

Page Size: US Letter

Reduction (%): 60

Synthesis/SYNLETT



Morphine

Fixed Length: 17 pt

Bold Width: 2 pt

Line Width: 0.8 pt

Margin Width: 1.3 pt

Hash Spacing: 2.5 pt

Chain Angle (degrees): 120

Bond Width (% of length): 18

Atom Label Font (Win/Mac): Arial/Helvetica

Atom Label Size: 10 pt

Caption Font (Win/Mac): Arial/Helvetica

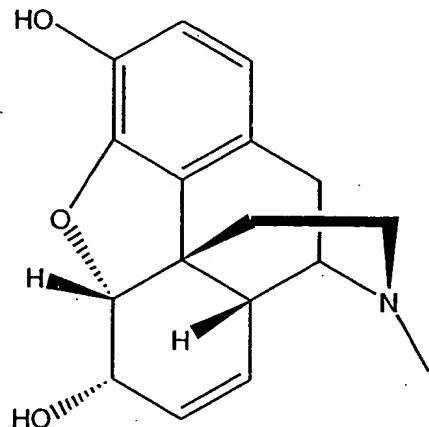
Caption Size: 10 pt

Drawing Area (Width x Height): 12 cm x 26.7 cm

Page Size: A4

Reduction (%): 100

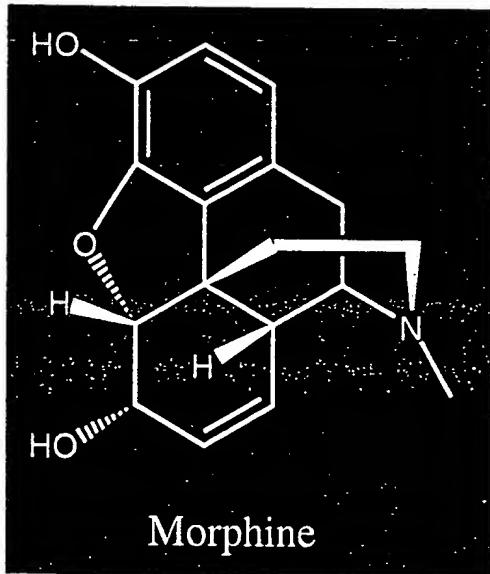
Table D-1 Drawing and Text (atom label and caption) Settings in Journal Style Sheets/Stationery Pads
(continued)



Morphine

New Document

Fixed Length: 30 pt
Bold Width: 2 pt
Line Width: 1 pt
Margin Width: 2 pt
Hash Spacing: 2.7 pt
Chain Angle (degrees): 120
Bond Width (% of length): 12
Atom Label Font (Win/Mac): Arial/Helvetica
Atom Label Size: 10 pt
Caption Font (Win/Mac): Times New Roman/Times
Caption Size: 12 pt
Drawing Area (Width x Height): 7.5 in x 10 in
Page Size: US Letter
Reduction (%): 100



Morphine

New Slide

Fixed Length: 30 pt
Bold Width: 4 pt
Line Width: 1.6 pt
Margin Width: 2 pt
Hash Spacing: 2.7 pt
Chain Angle (degrees): 120
Bond Width (% of length): 15
Atom Label Font (Win/Mac): Arial/Helvetica
Atom Label Size: 12 pt
Caption Font (Win/Mac): Times New Roman/Times
Caption Size: 16 pt
Drawing Area (Width x Height): 7.5 in x 10 in
Page Size: US Letter
Reduction (%): 100

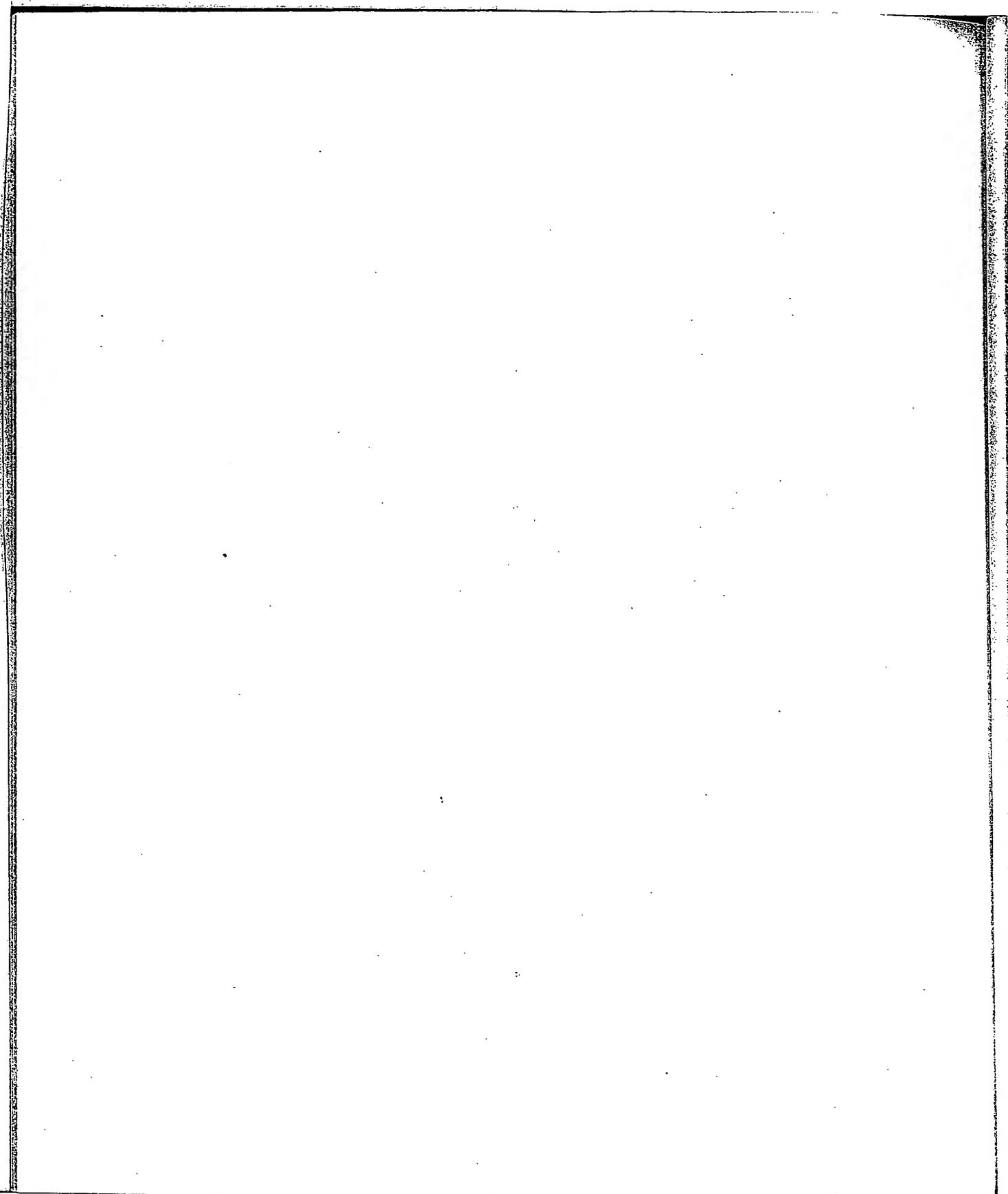
Appendix E, Apple Events (Macintosh)

ChemDraw supports Apple Events™, a method by which applications can send messages to each other. Using Apple Events it is possible to develop scripts for sequences of commands that can be executed repeatedly.

ChemDraw supports the Required Suite, a basic set of Apple Events that includes the Apple Events required to open and print documents from the Macintosh Finder.

ChemDraw supports the menu sharing Apple Events used in conjunction with Frontier, by Userland, Inc. Using Frontier, you can add items to the menu bar of *ChemDraw* that execute Frontier scripts.

For a complete technical specification of the Apple Events that *ChemDraw* supports, drag the *ChemDraw* application icon onto the Script Editor application icon or choose Open Dictionary from the Script Editor's File menu.



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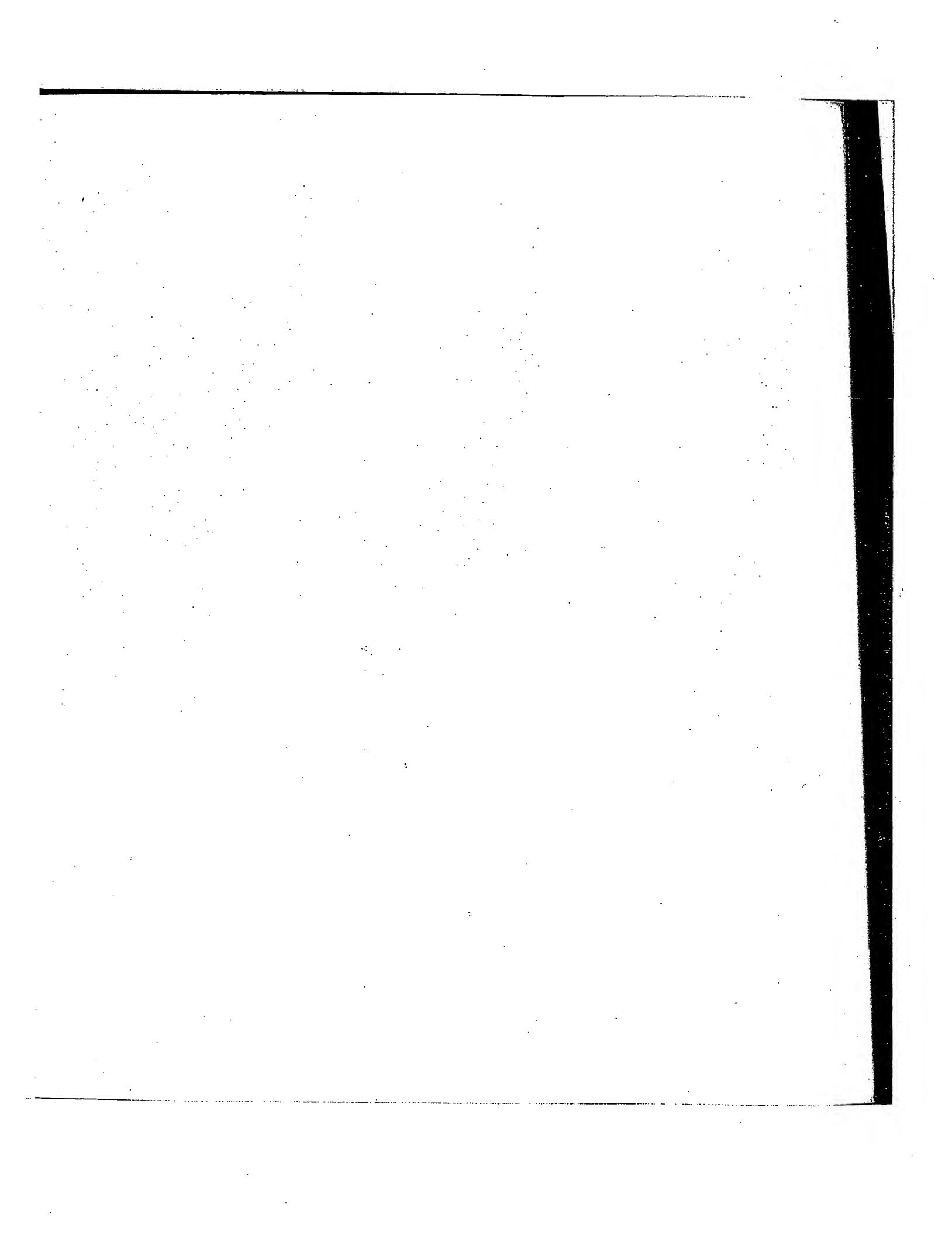
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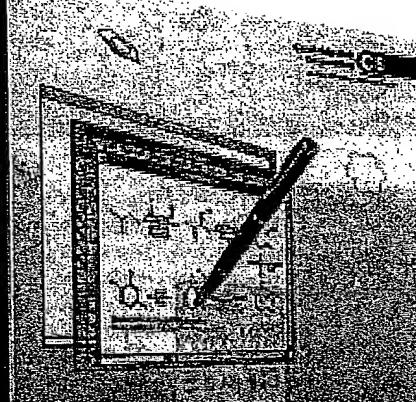
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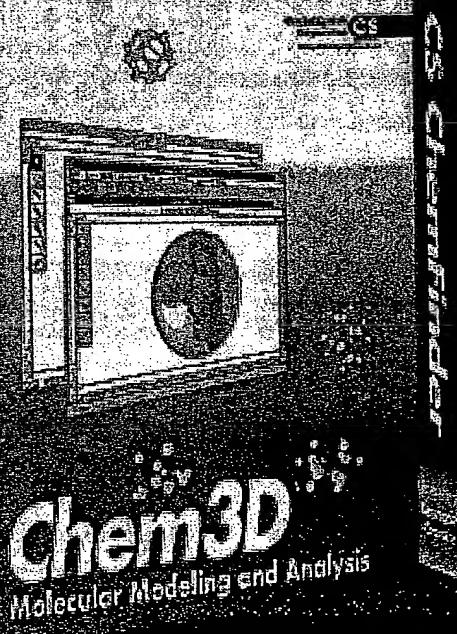
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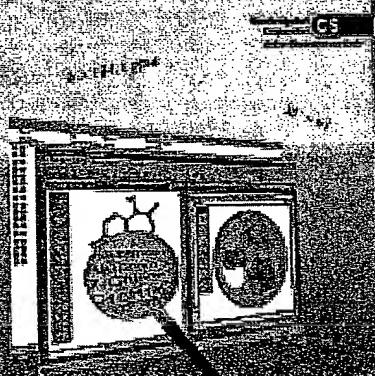
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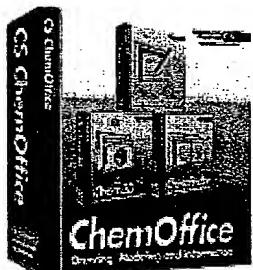
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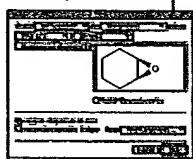
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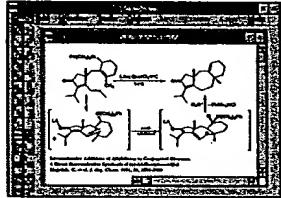
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Structure	Formula Molecular Weight Percent Weight
<chem>O=C1NC(=O)c2ccccc21</chem>	C ₁₁ H ₁₀ O ₂ 147.124 EC = 62.327 EW = 4.122 EW = 4.220 EW = 31.748

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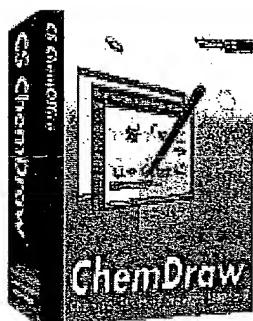
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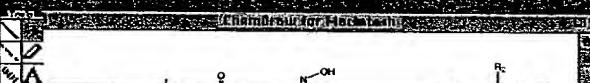
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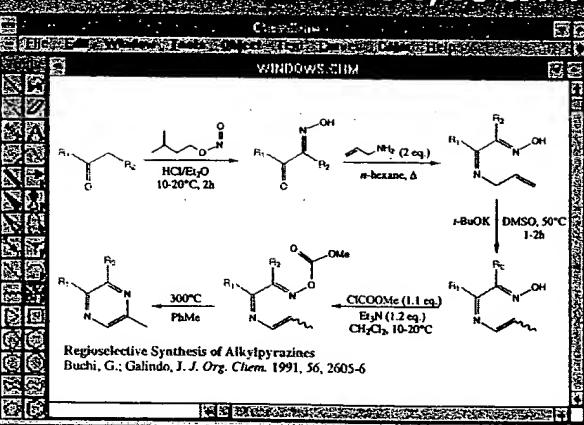
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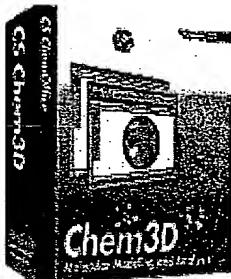
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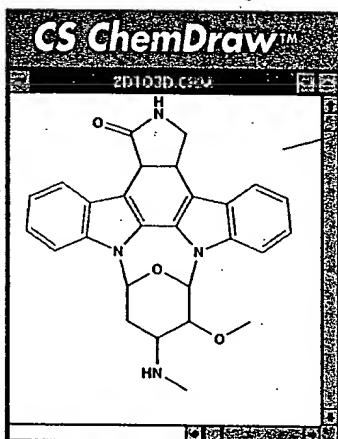
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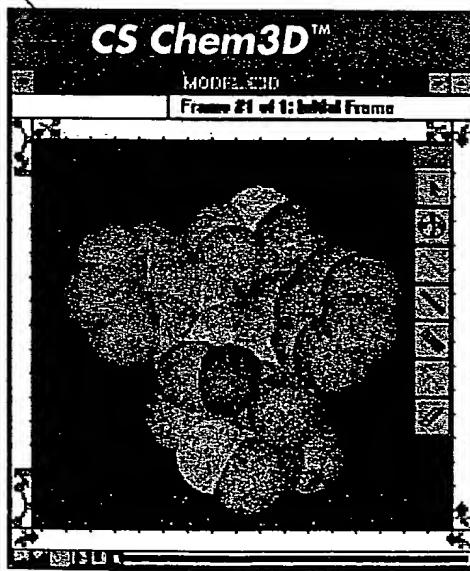
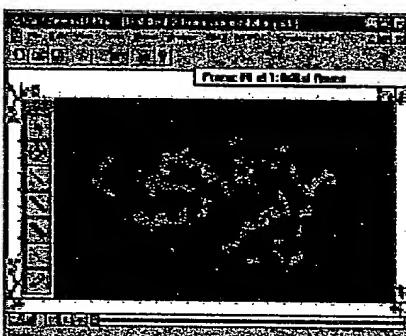
CS MOPAC Pro is a fully functional semi-empirical calculation engine that works with *Chem3D Pro*. **CS MOPAC Pro** computes properties, optimizes transition state and equilibrium geometries, and takes full advantage of the AM1, PM3, MNDO, and MINDO/3 potential functions.

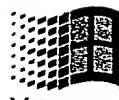
Complemented by *ChemDraw* and *ChemFinder* within *CS ChemOffice*, **CS Chem3D** and **CS MOPAC** demonstrate the power of 3D modeling seamlessly integrated with excellent chemical structure drawing, substructure searching and other information management tools.



With Chem3D, modeling in three dimensions is as easy as:

- 1 Draw structure in **ChemDraw** or ISIS/Draw
- 2 Cut & paste structure into **CS Chem3D**
- 3 3D model is automatically generated!




MICROSOFT
WINDOWS
COMPATIBLE
32-Bit Application

Macworld ★★★★☆

CS Chem3D Pro & MOPAC Pro

Premier Modeling, Visualization & Analysis

- Includes CS Chem3D Pro and CS MOPAC Pro
- Calculate ΔH_f , solvation energy, dipoles, charges, UHF and RHF spin densities
- Optimize transition state geometries
- AM1, PM3, MNDO, MINDO/3 methods
- Advanced MOPAC 93 engine

CS Chem3D Pro

Professional Modeling & Visualization

- Model types: ribbons, space filling (CPK), cylindrical bonds, ball & stick, and wire frame
- Display options: van der Waals dot surfaces; single-point light source color shading—*New*
- RasMol-like protein ribbons and sticks—*New*
- Create 3D models from ChemDraw or ISIS/Draw
- Polypeptide builder; residue recognition—*New*
- Real-time large molecule rotation—*New*
- Supports Brookhaven PDB, MacroModel, MDL MOLFILE, MSI MOLFILE, Chemical Abstracts via SMD, Beilstein ROSDAL (export), Tripos SYBYL MOL & MOL2, Cambridge Structural Database, MOPAC, EPS and PICT
- GIF format for WWW publishing—*New*

Computation and Analysis

- MM2 minimization and molecular dynamics
- Dock ligand and substrate molecules
- CS MOPAC Std included to optimize geometries with AM1, PM3, MNDO, and MINDO/3—*New*
- Calculate steric energy, bond lengths, interatomic distances, bond and torsional angles

Computational Add-Ons

- Interactive Simulations Sculpt® for real-time molecular modeling
- Dihedral driver and Monte Carlo conformational search—*Mac*
- Visual Basic OLE automation (Windows) and AppleScript (Mac)—*New*

Textbook & ChemOffice Ltd Bundles

- McGraw-Hill: *Organic Chemistry* (Carey)—*New*
- Saunders College Publishing: *Organic Chemistry* (Brown), *Biochemistry* (Garrett & Grisholm)

CS Chem3D Net

Advanced WWW Modeling Client

- Free academic and home use
- View, rotate and print models from WWW or disk
- Supports all Chem3D Pro display options
- Works with Netscape Navigator and NCSA Mosaic
- Available from <http://www.camsoft.com>

Platforms and Languages

Windows and Macintosh; English and Japanese
Windows: 386 or higher, 8MB Windows 3.1,
16MB Windows 95 or NT

Macintosh: 68020 or higher, or PowerMac, 8MB
CS MOPAC Pro requires PowerMac or Windows
and 8MB additional memory

All specifications subject to change without notice

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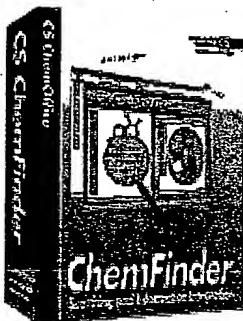
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CS ChemFinder™

Searching and Information Integration

NEW
ChemInfo

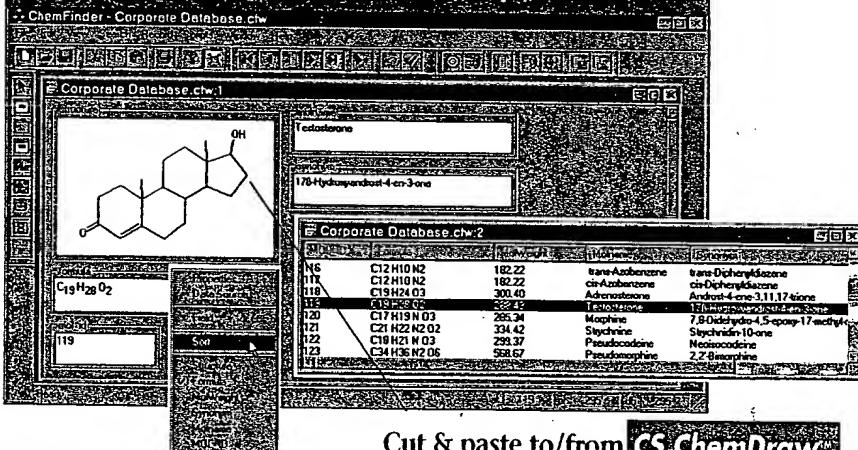


CS ChemFinder Pro is designed to organize all aspects of chemistry research, from the study of chemical structure to information about chemical compounds. In addition to being a complete personal chemical database, *ChemFinder* allows you to share your chemical data over intranets or the internet, and to query external chemical databases.

With *ChemFinder*, you can create customizable electronic laboratory notebooks, databases and forms. To organize a series of compounds, you simply draw the structures or models and paste them into *ChemFinder*. *ChemFinder's* intelligent database engine automatically computes the formula and molecular weight, and you can retrieve your data with a variety of easy searches. Teams of chemists use *ChemFinder* to manage projects, search literature, track laboratory chemicals (inventory), or connect their data to the WWW.

variety of easy searches. Teams of chemists use *ChemFinder* to manage projects, search literature, track laboratory chemicals (inventory), or connect their data to the WWW.

ChemFinder for Win 3.1, 95 & NT



ChemFinder - Corporate Database.cw

Corporate Database.cw:1

Testosterone

17^o-Hydroxyandrost-4-en-3-one

C₂₁H₂₈O₂

113

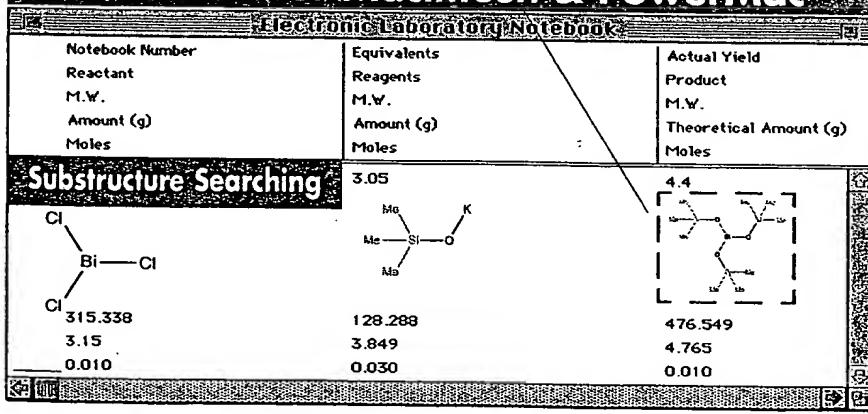
Corporate Database.cw:2

Number	Chemical Name	M.W.	Properties
106	C ₁₂ H ₁₀ N ₂	102.22	trans-Azobisisobutyronitrile
111	C ₁₂ H ₁₀ N ₂	102.22	cis-Azobisisobutyronitrile
118	C ₁₉ H ₂₄ O ₃	300.40	Adrenosterone
119	C ₁₉ H ₂₆ O ₃	322.42	Testosterone
120	C ₁₇ H ₁₉ N ₃ O ₂	265.34	Morphine
121	C ₁₇ H ₁₉ N ₃ O ₂	265.34	Strychnine
122	C ₁₉ H ₂₄ N ₂ O ₂	289.37	Pseudocodeine
123	C ₂₄ H ₃₆ N ₂ O ₆	558.67	Pseudomorphine

Cut & paste to/from CS ChemDraw™



ChemFinder for Macintosh & PowerMac



Electronic Laboratory Notebook

Notebook Number	Equivalents	Actual Yield
Reactant	Reagents	Product
M.W.	M.W.	M.W.
Amount (g)	Amount (g)	Theoretical Amount (g)
Moles	Moles	Moles

Substructure Searching

3.05

Cl
|
Bi—Cl
Cl
315.338
3.15
0.010

128.283
3.849
0.030

4.4

Me
|
Me—Si—O
Me

476.549
4.765
0.010

Macworld ★★★★

CS ChemFinder Pro

Premier Searching and Information

- Completely integrated with *ChemDraw* and *Chem3D*
- Store structures and models for easy retrieval
- Store physical and calculated data
- Search by substructure with stereochemical constraints
- Import data from *industry standard* SD file format
- Share group data across a network or the Internet
- World Wide Web Chemical Information Server included—*New*
- Annotate compounds with test results, notes, etc.
- Sort by formula, molecular weight, or any text or number field
- Automatically calculate molecular weight
- Convert 2D structures into 3D models
- Display detailed information by compound
- CS *ChemInfo Std* – a library of thousands of structures, models and information included

CS ChemFinder Pro for Windows

- Fully relational database engine—*New*
- Manages hundreds of thousands of compounds
- Simple, user-definable forms for custom displays
- High performance substructure searching
- Compound perception and search algorithms
- Connects to *Access*, *Oracle*, *Sybase* and other ODBC servers—*New*
- Information integration with *ChemOffice*, *Microsoft Office*, *GRAMS* and *Excel*
- Visual Basic OLE Automation, DDE and scripting
- Search by substructure, exact match or similarity

CS ChemFinder Pro for Macintosh

- Tabular data format for reference and calculations
- Calculate theoretical yield
- Search and store chemical reaction data
- Links with *Excel*, *FileMaker* and *4D* via AppleScript
- Access 6.3 million compound Beilstein database via *CrossFire*
- Access *Oracle* & *Sybase* relational databases
- Search *UNITY*, and *Chem-X* databases

Information Add-Ons

- ISI Index Chemicus 1995 data—*Windows*
- Marinlit marine chemistry data—*Mac*

Platforms and Languages

Windows and Macintosh; English and Japanese

Macintosh: System 7 or PowerPC, 12 MB

Windows: 386 or higher, 8MB Windows 3.1,

16MB Windows 95 or NT

All specifications subject to change without notice

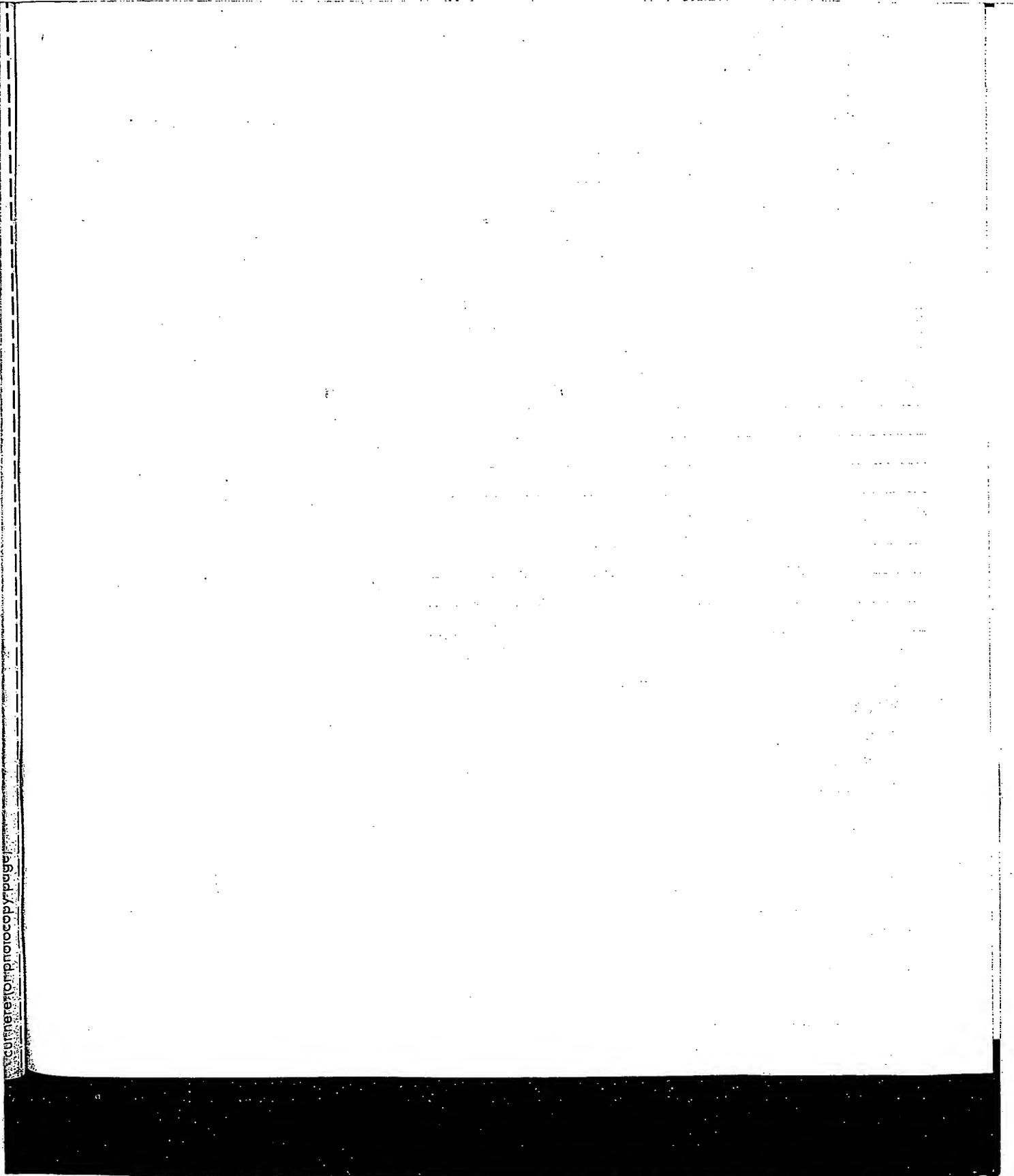
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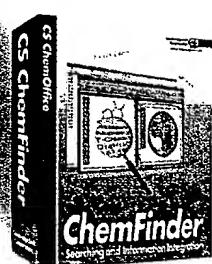
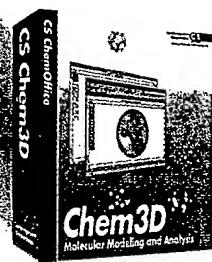
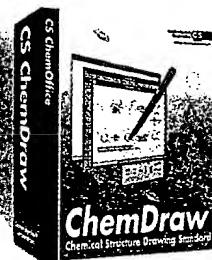
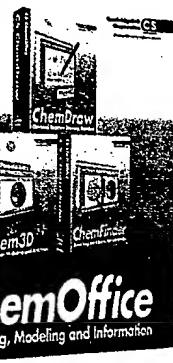
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CS ChemOffice™

Drawing, Modeling and Information



CS ChemOffice

unites *ChemDraw*,

Chem3D and *ChemFinder*

in an integrated suite that completely fulfills the day-to-day needs of chemists.

Draw any structure, instantly convert to 3D, and communicate your work quickly and easily. With *ChemOffice* the world of chemistry is only a few clicks away!

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